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ADAPTATION OF COMPUTER PROGRAM FOR POURBAIX DIAGRAMS TO
PERSONAL COMPUTERS(U) FLORIDA UNIV GAINESVILLE DEPT OF
MATERIALS SCIENCE AND ENGINEERING E D VERINK APR 83
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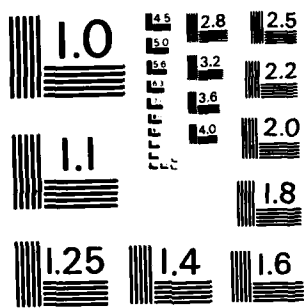
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AD A 128259

Final Report

Office of Naval Research
800 N. Quincy Street
Arlington, Virginia 22217

ADAPTATION OF COMPUTER PROGRAM FOR POURBAIX DIAGRAMS
TO PERSONAL COMPUTERS

Contract No. N00014-82-C-0718

Submitted by

Ellis D. Verink, Jr.

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University of Florida

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April 1983

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Final Report
ONR N00014-82-C0718

Since publication of Pourbaix's classic treatise "Atlas of Electrochemical Equilibria in Aqueous Solutions" (Pergamon Press, Oxford, CEBELCOR, Brussels, 1966), there has been interest in computerizing the calculation of Pourbaix diagrams in order to avoid the tedious task of calculating these diagrams "long-hand" for complex systems. Reference 1 reports a computerized method developed at University of Florida and currently in use in a number of laboratories which have access to main-frame computing facilities. On the assumption that personal computers can be made more readily available to scientists and engineers, there was interest in adopting the existing program for use on an Apple II personal computer.

ONR Contract #N00014-82-C0718 provided support for this effort. The new program developed at University of Florida has the following capabilities and advantages:

- (1) The program is written in UCSD-Apple Pascal which makes it adaptable to many microcomputer systems.
- (2) The method used to balance the equilibrium chemical equations allows the consideration of complicated metal-ion-water systems.
- (3) The program can be easily modified for high temperature applications through the inclusion of an available subprogram.
- (4) The method used to determine areas of predominance is intuitively obvious, rigorously correct, and continuum in its approach.
- (5) The program can be applied to determine equilibrium potential-pH diagrams for even very complex systems.



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The Program

The Fe-Cl-H₂O system provides a simple example of the application of the program. The metallic species which will be considered are shown in Table 1. Later, a more complex example will be given.

Table 1. DATA EMPLOYED IN COMPUTERIZED CALCULATION OF THE POTENTIAL vs pH DIAGRAM FOR THE Fe-Cl-H₂O SYSTEM AT 25°C

Species considered		Gibb's free energy of formation (in cal/M)	Assumed thermodynamic activity
Chemical notation	Computer notation		
Cl-	CL-	-31372.0	1.0 x 10 ⁻¹
Fe	FE	0.0	1.0
Fe ₃ O ₄	FE304	-242700.0	1.0
Fe ₂ O ₃	FE203	-177400.0	1.0
HFeO ₂ ⁻	HFE02-	-90300.0	1.0 x 10 ⁻⁶
FeOH ²⁺	FE0H++	-54830.0	1.0 x 10 ⁻⁶
Fe(OH) ₂ ⁻	FE(OH)2+	-104700.0	1.0 x 10 ⁻⁶
FeCl ₂ (Aq)	FECL2(AQ)	-81590.0	1.0 x 10 ⁻⁶
FeCl ²⁺	FECL++	-34400.0	1.0 x 10 ⁻⁶

Since computer line printers display only capital letters, it is necessary to develop a suitable convention for writing chemical equations entirely on one line (no subscripts) and in capital letters. Any reasonable, internally consistent, convention may be employed. Further reference to Table 1 will supply insight into the type of convention employed by the authors in this example. In order to avoid confusion in reading the balanced chemical equations, the computer places an asterisk between all coefficients and the chemical species to which they refer.

Input of Data

Data is entered into the microcomputer interactively. The user is prompted for each piece of data to be entered. In order to prevent crashing, all data is read as characters and converted to integer or real values as required.

The first piece of data to be entered is the temperature, in degrees Kelvin, to be used in Nernst equation calculations. Temperature corrections of free energy data may be done using a separate subprogram based on the methods of Criss & Cobble. (ref. 2)

The number of non-metallic ionic species to be considered is entered. In this example the number 1 is entered, since only Cl^- is considered. Pertinent ionic-species data in the form of each species' name, free energy of formation, activity, electrical charge and elemental composition is then input.

Immediately after the ionic species data the number of metallic species to be considered is entered (for the Fe-Cl- H_2O system this number is 8, since Cl^- would not be counted as a metallic species). Other pertinent data similar to that listed above for the ionic species is then input for each metallic species.

When data entry is completed the user is asked if the data requires correction. The user is able to select and modify any piece of data.

The data is written to the terminal or printer as specified by the user. The tabular form allows checking for accuracy and the user is again offered the opportunity to modify the entered data.

Chemical equation balancing and Equilibrium Line Determination

When considering the possible formation of N different metallic species

$$\frac{N(N-1)}{2}$$

chemical equilibrium equations exist. The program balances chemical equations between all of the possible pairs of metallic species. The program takes all possible pairs of metallic species and balances the equations in terms of water, hydrogen ions, electrons, etc. The balanced chemical equations are used by the computer to determine and tabulate the equilibrium line equations by means of Nernst equation calculations.

(For a simple explanation of the calculations involved, consult Ref. 3)

Areas of Predominance

Determining the areas of predominance on a potential-pH diagram requires a proper understanding of the information conveyed by each line on the diagram. Each line represents equilibrium coexistence between two metallic species (with certain assumptions regarding ionic activities). When any line is crossed one metallic species becomes more energetically favorable than another. Each line, therefore, delineates a boundary between two adjacent areas on the diagram. Each area represents the region (in potential vs pH coordinates) in which a particular species is thermodynamically stable and dominant. By simultaneously considering all of the lines which correspond to equilibria involving a given species, an area is traced out in which the species in question is "not excluded". This then is the area of predominance for that species.

When each species is considered (one at a time) in the above manner, a series of separate areas of predominance results. When these separate areas are fitted together, they form the finished theoretical potential-pH diagram without any overlaps.

A mathematical analog can be drawn by considering the equilibrium lines as inequalities. For example, in considering the equilibrium between Fe and Fe_3O_4 , Fe is the predominant species at values of potential and pH less than those described by the equilibrium coexistence line between Fe and Fe_3O_4 (hence the term "inequality"). Thus a given species will exist whenever the potential and pH satisfy all of the line inequalities pertaining to the species. If no potential and pH simultaneously satisfies all of the inequalities of a given species, the species has no area of predominance.

The field of operations research has been developed by industrial and systems engineers to deal with such mathematical analogs. In operations research the area which mutually satisfies a set of linear inequalities is termed a "convex polygon".* Methods of determining convex polygons, therefore, lend themselves to determining areas of predominance on potential-pH diagrams.

Computer determination of areas of predominance

The equation balancing portion of the program is designed to write all electron-transfer equations as oxidation reactions. This results in

* Convex polygon—an area such that if a line segment is drawn between any two arbitrarily selected points in the polygon all points on the line segment will also lie within the polygon. (Ref. 3)

two important consequences. First, for all constant-pH lines the metallic species on the lower pH (left) side of the line will appear on the left side of the chemical equation. Second, for all non-vertical lines the metallic species which lie on the lower potential sides of the lines will also be on the left side of the chemical equation. By noting whether the various lines are vertical or nonvertical and on which side of the chemical equations the species occur, lines can be sorted into the following four categories: (1) minimum pH lines; (2) maximum pH lines; (3) potential, upper bound lines; and (4) potential, lower bound lines. The program uses this sorting technique to determine the convex polygon for each metallic species which simultaneously satisfies all the equilibrium line equations of each individual species. The resulting polygons are displayed to the user by the computer as a set of points which constitute the corners of each convex polygon. Plotting the determined points (expressed in potential and pH coordinates) and connecting them with straight lines results in a diagram like the one shown in Fig.

1 for Fe-Cl-H₂O.

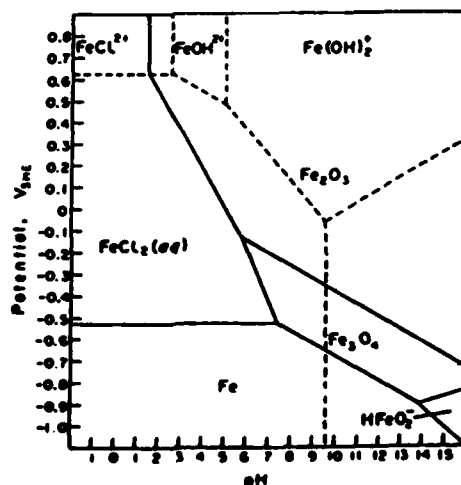


FIG. 1. Potential vs pH diagram for the Fe-Cl-H₂O system at 25°C as determined by computer considering the species shown in Table 1.

Determination of more Complex Systems

More complex metal-ion-water systems involving ionic species which

Calculation of potential-pH diagrams of metal-ion-water systems by computer

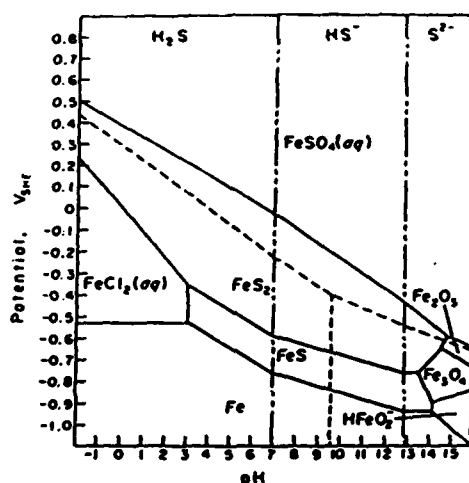


FIG. 2. Potential vs pH diagram for the Fe-Cl-S-H₂O system at 25°C as determined by the computer considering the species shown in Tables 1 and 2.

have their own potential-pH equilibria (e.g. H₂S, HS⁻, S²⁻) appear to violate the previous theory for determining regions of predominance.

Such is not the case when the program is properly employed.

Addition of the species shown in Table 2 to those in Table 1 results in the computer determined diagram shown in Fig. 2. Note even though the region of predominance for FeS does not, as a whole, constitute a convex polygon, the portions of the region which lie in each of the individual areas of predominance for H₂S, HS⁻ and S²⁻ respectively, are in each case convex. Thus when it becomes necessary to formulate such a diagram it requires the initial computer calculation of more than

one diagram. In this case three diagrams were determined considering individually H_2S , HS^- and S^{2-} . The appropriate portion of each of the three diagrams was then used to construct the final diagram

Table 2. DATA EMPLOYED IN COMPUTERIZED CALCULATION OF THE POTENTIAL vs pH DIAGRAM FOR THE Fe-Cl-S SYSTEM AT 25°C

Species considered		Gibb's free energy of formation (in cal/M)	Assumed thermodynamic activity
Chemical notation	Computer notation		
H_2S	H2S	-6660.0	1.0×10^{-1}
HS^-	HS-	2880.0	1.0×10^{-1}
S^{2-}	SS--	20500.0	1.0×10^{-1}
FeS (Solid)	FES (SOL)	-24000.0	1.0
FeS_2 (Solid)	FES2 (SOL)	-39900.0	1.0
FeSO_4 (Aq)	FESO4 (AQ)	-196820.0	1.0×10^{-6}

shown in Fig. 2 taking into account the domain of stability of each ionic species. (For simplicity the diagrams are drawn with straight-line segments meeting at the "equal dominance" lines for adjacent ionic species. Actually at such lines (e.g. $\text{HS}^-/\text{S}^{2-}$) the activities of both species are equal at the equal dominance line but one species rapidly predominates as one moves away from the line.) Using this technique even more complicated systems can be determined.

Summary of Program Capabilities

The interactive microcomputer version of the pH potential program is largely a translation of the WATFIV version and takes advantage of UCSD Pascal features.

The described computer program is arbitrarily designed to consider a maximum of 35 metallic species and 10 non-metallic ionic species simultaneously. Redimensioning of the program matrices will allow for any desired increase or decrease in the program's capacity.

The structure of the program and the UCSD operating system facilitate the addition of extensions to the program through the independent development of new modules. It is hoped that support can be obtained for development of additional modules including a data maintenance routine that will record on disk a library of data for selected metal-ion-water systems and an accompanying graphics package that will permit interactive terminal and printer output of generated pH potential diagrams.

REFERENCES

1. M. H. Froning, M. E. Shanley, and E. D. Verink. "An Improved Method for Calculation of Potential -pH Diagrams of Metal-Ion-Water Systems by Computer", Corrosion Science, 1976, Vol. 16, pp. 371-377.
2. C. M. Criss and J. W. Cobble. J. Am. Chem. Soc., 86, 5394 (1964).
3. E. D. Verink, "Simplified Procedure for Constructing Pourbaix Diagrams" JEMSE, Vol. 1, No. 3, Fall 1979, pp. 535-560.
4. H. M. Wagner, Principles of Operations Research, pg. 83, Prentice-Hall, N.J. (1969).

Attachments Include:

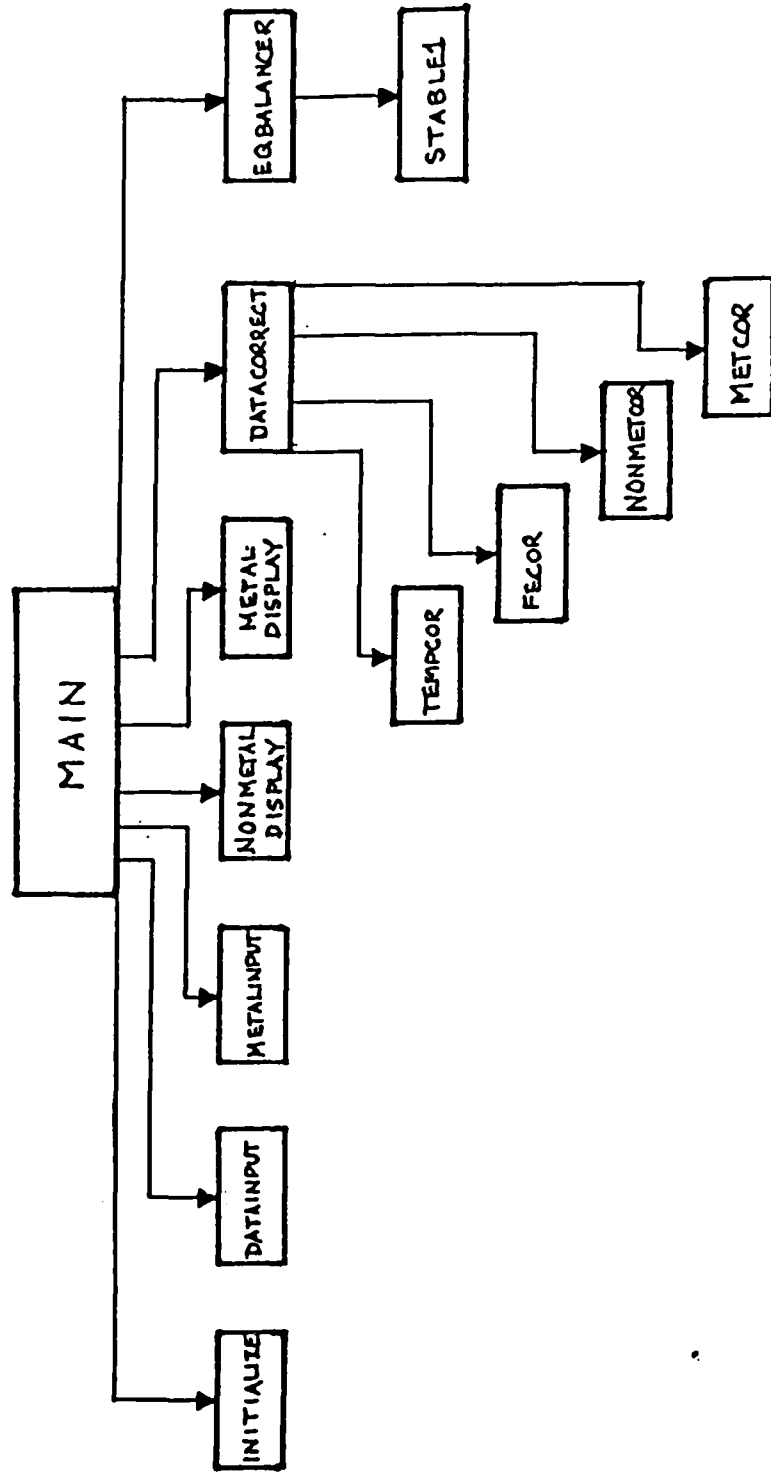
Flow chart

Modular Documentation

The Main Program with Accompanying Units

User's Guide

Example of Output



FLOW DIAGRAM OF PRIMARY PROGRAM MODULES

PH - POTENTIAL PROGRAM

MODULAR DOCUMENTATION

MODULAR DESCRIPTION FORM

- A. MODULAR NAME - Metal input (* part of unit in data*)
- B. MODULE FUNCTION - Prompts user for metallic species data
- C. INPUTS (ARGUMENTS, COMMON, FILE & TERMINAL) - Terminal: Number of metallic species (NP)
Name of metallic specie (SP [M, HH])
Free energy of formation (F [M])
Ionic activity (AM [M])
Electrical charge (Z [M])
Number of metal atoms (Metal [M])
Number of oxygen atoms (Oxygen [M])
Number of hydrogen atoms (Hydro [M])
Number of characteristic atoms for each ionic species (ION [I, M])
- D. OUTPUTS (ARGUMENTS, COMMON, FILE & TERMINAL) - None
- E. SUMMARY OF PROCESS - Sequentially prompts user for metallic species data. All real values read as characters by the procedure inreal, and are converted to real by CHAR to REAL. Integer values are also read as characters and are converted to integer by CHAR to INT. Name of species is read in by the procedure GETMET.
- F. CALLS THESE MODULES - Procedures: INCHAR, INREAL, GETMET, LF.
Unit: Convert
- G. CALLED BY THESE MODULES - Main

MODULAR DESCRIPTION FORM

- A. MODULAR NAME - Data input (* part of unit in data *)
- B. MODULE FUNCTION - Prompts user for non-metallic ionic species data
- C. INPUTS (ARGUMENTS, COMMON, FILE & TERMINAL) - Terminal:Temperature (T)
Free energy of formation of H_2O (FEH₂O)
Number of non-metallic ions (NION)
Name of species (Name [K, HH])
Free energy of formation (FION [1])
Ionic activity (AION [1])
Electrical charge (ZION [1])
Number of characteristic atoms (BION [1])
Number of Oxygen atoms (OXY [1])
Number of hydrogen atoms (HYD [1])
- D. OUTPUTS (ARGUMENTS, COMMON, FILE & TERMINAL) - None
- E. SUMMARY OF PROCESS - Sequentially prompts user for non-metallic ionic species data. All real values are read as characters by the procedure inreal and converted to real by CHAR to REAL. Integer values are also read as characters and are converted to integers by CHAR to INT. Name of species is read by the procedure GETNONMET.
- F. CALLS THESE MODULES - Procedures:INCHAR, INREAL, GETNONMET, LF.
Unit:Convert.
- G. CALLED BY THESE MODULES - Main

MODULAR DESCRIPTION FORM

- A. MODULAR NAME - Initialize**
- B. MODULE FUNCTION - Initialization of index values, ionic species values, and species name array**
- C. INPUTS (ARGUMENTS, COMMON, FILE & TERMINAL) - None**
- D. OUTPUTS (ARGUMENTS, COMMON, FILE & TERMINAL) - None**
- E. SUMMARY OF PROCESS - Initializes program counter index to 1. Initializes FION [1], OXY [1], to 0. Initializes S, Name, X, SP to all blanks ("b").**
- F. CALLS THESE MODULES - None**
- G. CALLED BY THESE MODULES - Main**

MODULAR DESCRIPTION FORM

- A. MODULAR NAME - Main program
- B. MODULE FUNCTION - Controls execution of program
- C. INPUTS (ARGUMENTS, COMMON, FILE & TERMINAL) - Interactively prompts user for display option (printer or terminal)
- D. OUTPUTS (ARGUMENTS, COMMON, FILE & TERMINAL) - None
- E. SUMMARY OF PROCESS - Sequentially calls primary program modules for:
 - 1. input of data
 - 2. correction of data
 - 3. display of data
 - 4. correction of data
 - 5. equation balancing
- F. CALLS THESE MODULES - Initialize, data input, metal input, nonmetal display, metal display, data correct, Bq balancer
- G. CALLED BY THESE MODULES - None

MODULAR DESCRIPTION FORM

- A. MODULAR NAME - Stable 1 (* part of unit stable *)
- B. MODULE FUNCTION - Determining areas of predominance
- C. INPUTS (ARGUMENTS, COMMON, FILE & TERMINAL) - None
- D. OUTPUTS (ARGUMENTS, COMMON, FILE & TERMINAL) - Listing of areas of predominance, line segment data. Listing of minimum and maximum constant pH line data.
- E. SUMMARY OF PROCESS - Determine minimum pH line for metallic species (Stable 3). Determines maximum constant pH line for metallic species (Stable 4). Calculates upper bound lines to determine the line which supplies minimum potential for upper bound of stability region at minimum pH (UPBNDLNS). Calculates intersection points between previously determined upper bound lines and remaining upper bound lines (INTPTS HI). Calculates lower bound lines (LOWBNDLNS) and intersection points for lower bound lines (INTPTS LO). Tests upper and lower bounds to determine whether they intersect within the minimum and maximum pH lines. If they intersect, the points are determined and data is printed. Orders pH values at which either two upper bound lines or two lower bound lines intersect from PHMIN to PHMAX. Finds point where upper bound exceeds lower bound. Determines intersection point on maximum pH side. Prints data.
- F. CALLS THESE MODULES - Procedures: Start, Set flags, Stable 2, Stable 3, Stable 4, UPBNDLNS, INTPTS HI, TEMP 1, LOWBNDLNS, INTPTS LO, TEMP 2, Stable 5, Stable 6, Stable 7, Stable 8, Stable 9, Stable 10, Stable 11.
- G. CALLED BY THESE MODULES - Eq Balancer

MODULAR DESCRIPTION FORM

- A. MODULAR NAME - Eq Balancer
- B. MODULE FUNCTION - Balances equations between all possible pairs of metallic species.
- C. INPUTS (ARGUMENTS, COMMON, FILE & TERMINAL) - None
- D. OUTPUTS (ARGUMENTS, COMMON, FILE & TERMINAL) - Terminal or Printer: Balanced equations. Equilibrium line equation.
- E. SUMMARY OF PROCESS - Balances chemical equations between all possible pairs of metallic species. Takes all pairs of metallic species and balances them in terms of water, hydrogen ions, electrons, etc. NERNST equation calculations are then used to tabulate the equilibrium line equations. Procedure diagram then calls stable 1.
- F. CALLS THESE MODULES - Procedures:EQB1, SUMNUM, Update, LOGSUM, FINDSIGN, EQB4, CALCEQEQ, Diagram, Stable 1.
- G. CALLED BY THESE MODULES - Main

MODULAR DESCRIPTION FORM

- A. MODULAR NAME - Nonmetcor (* part of unit in data *)
- B. MODULE FUNCTION - Correction of non-metallic species data entered.
- C. INPUTS (ARGUMENTS, COMMON, FILE & TERMINAL) - Terminal: Parameter to be modified. (Name, FION, AION, ZION, BION, OXY, HYD). New value for parameter specified.
- D. OUTPUTS (ARGUMENTS, COMMON, FILE & TERMINAL) - Terminal: Menu of parameters. Old value of parameter.
- E. SUMMARY OF PROCESS - Asks which ion to modify. Displays menu of options to be modified.
1. ion name
 2. free energy of formation
 3. activity
 4. charge
 5. number of characteristic atoms
 6. number of oxygen atoms
 7. number of hydrogen atoms

Writes old value of parameter, prompts for and reads new value.

F.CALLS THESE MODULES - Procedures:NMETC1, NMETC2, NMETC3, NMETC4, NMETC5, NMETC6, NMETC7, 6ETNONMET, INREAL, INCHAR.
Unit:Convert

G.CALLED BY THESE MODULES - Data correct

MODULAR DESCRIPTION FORM

A. MODULAR NAME - Metcor

B. MODULE FUNCTION - Correction of metallic species data entered.

C. INPUTS (ARGUMENTS, COMMON, FILE & TERMINAL) - Terminal:species and parameter to be modified (SP, F, AM, Z, Metal, Oxygen, Hydro, Ion).

New value for parameter specified.

D. OUTPUTS (ARGUMENTS, COMMON, FILE & TERMINAL) - Terminal:Menu of parameters. Old value of parameter.

E. SUMMARY OF PROCESS - Asks for species to be modified. Displays menu of options.

1. specie name
2. free energy of formation
3. activity
4. charge
5. number of metal atoms
6. number of oxygen atoms
7. number of hydrogen atoms
8. number of characteristic atoms

Writes old value of parameter, prompts for and reads new value.

F.CALLS THESE MODULES - Procedures:METC1, METC2, METC3, METC4, METC5, METC6, METC7, METC8, GETMET, INCHAR, INREAL.
Unit:Convert

G.CALLED BY THESE MODULES - Data correct.

MODULAR DESCRIPTION FORM

- A. MODULAR NAME - Fecor (* part of unit in data *)
- B. MODULE FUNCTION - Correction of free energy of formation of H_2O entered.
- C. INPUTS (ARGUMENTS, COMMON, FILE & TERMINAL) - Terminal: FEH_2O
- D. OUTPUTS (ARGUMENTS, COMMON, FILE & TERMINAL) - Old FEH_2O value
- E. SUMMARY OF PROCESS - Prints current value of FEH_2O . Prompts for and reads new value of FEH_2O .
- F. CALLS THESE MODULES - Procedure: Inreal
Unit: Convert
- G. CALLED BY THESE MODULES - Data correct

MODULAR DESCRIPTION FORM

- A. MODULAR NAME - Tempcor
- B. MODULE FUNCTION - Correction of temperature entered
- C. INPUTS (ARGUMENTS, COMMON, FILE & TERMINAL) - Terminal: T
- D. OUTPUTS (ARGUMENTS, COMMON, FILE & TERMINAL) - Old T value
- E. SUMMARY OF PROCESS - Prints out current value of temperature.
Prompts for and reads new value of temperature.
- F. CALLS THESE MODULES - Procedure:Inreal
Unit:Convert
- G. CALLED BY THESE MODULES - Data correct

MODULAR DESCRIPTION FORM

- A. MODULAR NAME - Data correct (* part of unit in data *)
- B. MODULE FUNCTION - User correction of data entered
- C. INPUTS (ARGUMENTS, COMMON, FILE & TERMINAL) - Data type to be modified (Opt.)
- D. OUTPUTS (ARGUMENTS, COMMON, FILE & TERMINAL) - None
- E. SUMMARY OF PROCESS - Prompts user for type of data that requires modification. The options are:
1. temperature
 2. free energy of H₂O
 3. non-metallic species data
 4. metallic species data
 5. data is now correct
- Calls appropriate procedure.
- F. CALLS THESE MODULES - Procedures: Tempcor, Fecor, Nonmetcor, Metcor
- G. CALLED BY THESE MODULES - Main

MODULAR DESCRIPTION FORM

- A. MODULAR NAME - Metal display
- B. MODULE FUNCTION - Displays metallic species data
- C. INPUTS (ARGUMENTS, COMMON, FILE & TERMINAL) - None
- D. OUTPUTS (ARGUMENTS, COMMON, FILE & TERMINAL) - Terminal or
Printer: SP, F, AM, Z, Metal, Oxygen, Hydro, Ion
- E. SUMMARY OF PROCESS - Displays metallic species data in tabular form
to terminal or printer as specified by user.
- F. CALLS THESE MODULES - Procedures: Dis 1 MET, Dis 2 MET, Dis 3 MET,
Draw.
- G. CALLED BY THESE MODULES - Main

MODULAR DESCRIPTION FORM

- A. MODULAR NAME - Nonmetal display
- B. MODULE FUNCTION - Displays non-metallic species data
- C. INPUTS (ARGUMENTS, COMMON, FILE & TERMINAL) - None
- D. OUTPUTS (ARGUMENTS, COMMON, FILE & TERMINAL) - Terminal or
Printer: T, FEH20, Name, FION, AION, ZION, BION OXY, HYD
- E. SUMMARY OF PROCESS - Displays non-metallic species data in tabular
form to terminal or printer as specified by user.
- F. CALLS THESE MODULES - Procedures: ions out 1, ions out 2, draw.
- G. CALLED BY THESE MODULES - Main

```

(*$S+*)
PROGRAM PHPOTENTIAL(INPUT,OUTPUT);

USES TRANSCEND,GETVALUE,CONVERT,INDATA,STABLE;
TYPE
  AONAME  =ARRAY[1..15,1..15] OF CHAR;
  MATRIX80=ARRAY[1..80] OF CHAR;
  AOINT10 =ARRAY[1..10] OF INTEGER;
  MAR2X595=ARRAY[1..2] OF ARRAY[1..595] OF REAL;
  AOCH15  =ARRAY[1..15] OF CHAR;

VAR
  C,COEF      :AOI15;
  JINDEX,INDEX:INTEGER;
  MUN,A,NPP   :INTEGER;
  NUMB,NUM,NUME:INTEGER;
  II,HH,KK    :INTEGER;
  J,K,L,I,M   :INTEGER;
  IONS,NONION  :INTEGER;
  SAVE,TEMP,S  :AOCH15;
  MAT          :MATRIX80;
  X            :AONAME;
  NUMF,SUMAIO  :REAL;
  ACT,ACT1,ACT2:REAL;
  DELC,PH      :REAL;
  HE,ZAP1,ZAP2 :REAL;
  EN,ZAP3,ZAP4 :REAL;
  OPT1,NOPT    :CHAR;
  AB           :BOOLEAN;

PROCEDURE INITIALIZE;
BEGIN
  INDEX:=1;
  FION[1]:=0.0;
  AION[1]:=1.0;
  ZION[1]:=0;
  BION[1]:=0;
  OXY[1]:=0;
  HYD[1]:=0;
  FOR I:=1 TO 15 DO
    BEGIN
      S[I]:=' ';
      FOR J:=1 TO 15 DO
        BEGIN
          NAME[I,J]:=' ';
          X[I,J]:=' ';
        END;
      END;
      FOR I:=1 TO 35 DO
        FOR J:=1 TO 15 DO
          SPC[I,J]:=' ';
        END;
      END;
    END;

PROCEDURE FINDSIGN;
BEGIN
  FOR J:=1 TO NUMB DO
    IF COEF[J]<>0 THEN
      BEGIN
        I:=I+1;
        S[I]:='+';
        IF I=1 THEN S[I]:=' ';
        IF COEF[J]<0 THEN S[I]:='-';
        IF J=(NION+3) THEN
          BEGIN
            S[I]:='=';
            C[I]:=COEF[J];
          END
        ELSE C[I]:=ABS(COEF[J]);
        FOR HH:=1 TO 15 DO X[I,HH]:=NAME[J,HH];
      END;
    END;
  END;

```

```

PROCEDURE UPDATE;
BEGIN
  FOR I:=1 TO NUMB DO
    COEF[I]:=-COEF[I];
    J:=COEF[I];
    FOR HH:=1 TO 15 DO
      BEGIN
        NAME[I,HH]:=NAME[NION+3,HH];
        NAME[NION+3,HH]:=TEMP[HH];
      END;
    COEF[I]:=-COEF[NION+3];
    COEF[NION+3]:=-J;
    ACT:=ACT1;
    ACT1:=ACT2;
    ACT2:=ACT;
    LINE[1,MI]:=A;
    LINE[2,MI]:=M;
    DELG:=-DELG;
  END;
END;

PROCEDURE SUMNUM;
BEGIN
  MUN:=0;
  NUM:=0;
  NUMF:=0;
  FOR I:=1 TO NION DO
    BEGIN
      NUM:=NUM+COEF[I+2]*OXY[I];
      MUN:=MUN+COEF[I+2]*HYD[I];
      NUMF:=NUMF+COEF[I+2]*FION[I];
    END;
    COEF[2]:=OXYGEN[A]*METAL[M]-OXYGEN[M]*METAL[A]-NUM;
    COEF[NION+4]:=COEF[2]*2-HYDRO[A]*COEF[NION+3]+HYDRO[M]*COEF[1]+MUN;
    DELG:=COEF[NION+3]*F[A]-COEF[1]*F[M]-COEF[2]*FEH2O-NUMF;
    NUME:=0;
    FOR I:=1 TO NION DO
      NUME:=NUME+COEF[I+2]*ZION[I];
    COEF[NION+5]:=COEF[NION+4]-NUME-COEF[1]*Z[M]+COEF[NION+3]*Z[A];
  END;
END;

PROCEDURE EQWRITE;
BEGIN
  KK:=1;
  WHILE MAT[KK]<>'*' DO
    BEGIN
      WRITE(FF,MAT[KK]);
      KK:=KK+1;
      IF MAT[KK]='*' THEN
        BEGIN
          WRITELN(FF,MAT[KK]);
          KK:=KK+1;
          WRITE(FF,' ');
          WRITE(FF,' ');
        END;
      END;
    END;
  LNFD(1);
  WRITELN(FF,' ');
END;

PROCEDURE SUB10;
BEGIN
  LTYPE[MI]:=0;
  EQUAT[1,MI]:=0;
  EQUAT[2,MI]:=0;
  WRITE(FF,' ',MI:3,' ',! NO LINE GENERATED');
  WRITE(FF,' ');
  EQWRITE;
END;

PROCEDURE SUB11;
BEGIN
  ZAP1:=DELG/(2.303*1.987*T);
  ZAP2:=COEF[NION+3]*LOG(ACT2);
  ZAP3:=COEF[1]*LOG(ACT1);
  PH:=(ZAP1+ZAP2-ZAP3-SUMA10)/COEF[NION+4];
  LTYPE[MI]:=1;
  EQUAT[1,MI]:=PH;
  EQUAT[2,MI]:=0;
  WRITE(FF,' ',MI:3,' ',! PH=' ',PH:8:2);
  WRITE(FF,' ');
  EQWRITE;
END;

```

```

PROCEDURE CALCEQEQ;
BEGIN
  IF (COEF[NION+5]=0) AND (COEF[NION+4]=0) THEN SUB10
  ELSE
    IF COEF[NION+5]=0 THEN SUB11
    ELSE
      BEGIN
        ZAP1:=1.9844*T/COEF[NION+5];
        ZAP2:=DELG/(COEF[NION+5]*23060.0);
        ZAP3:=COEF[NION+3]*LOG(ACT2);
        ZAP4:=COEF[1]*LOG(ACT1);
        HE:=- (COEF[NION+4]*ZAP1*0.0001);
        EN:=ZAP2+ZAP1*(ZAP3-ZAP4-SUMAIO)*0.0001;
        LTYPE[M1]:=2;
        EQUAT[1,M1]:=EN;
        EQUAT[2,M1]:=HE;
        IF HE=0 THEN
          BEGIN
            WRITE(FF,' ',MI:3,' ',E=' ',EN:8:4);
            WRITE(FF,' ');
            EQWRITE;
          END
        ELSE
          IF HE<0 THEN
            BEGIN
              HE:=-HE;
              WRITE(FF,' ',MI:3,' ',E=' ',EN:8:4);
              WRITE(FF,' - ',HE:7:4,'PH ');
              EQWRITE;
            END
          ELSE
            BEGIN
              WRITE(FF,' ',MI:3,' ',E=' ',EN:8:4);
              WRITE(FF,' + ',HE:7:4,'PH ');
              EQWRITE;
            END
          END;
        END;
      FOR KK:=1 TO 80 DO MAT[KK]:=' ';
      FOR KK:=1 TO 15 DO NAME[1,KK]:=TEMP[KK];
    END;
  END;

```

```

PROCEDURE EQB4;
BEGIN
  FOR KK:=1 TO 80 DO MAT[KK]:=' ';
  II:=1;
  FOR J:=1 TO I DO
    BEGIN
      IF J<>1 THEN
        BEGIN
          MAT[II]:=S[J];
          II:=II+1;
          MAT[II]:=' ';
          II:=II+1;
        END;
      IF C[J]<>1 THEN
        BEGIN
          GETVAL(C[J],SAVE);
          FOR KK:=1 TO 15 DO
            IF SAVE[KK]<>' ' THEN
              BEGIN
                MAT[II]:=SAVE[KK];
                II:=II+1;
              END;
          MAT[II]:='*';
          II:=II+1;
        END;
      FOR KK:=1 TO 15 DO
        SAVE[KK]:=X[J,KK];
      FOR KK:=1 TO 15 DO
        IF SAVE[KK]<>' ' THEN
          BEGIN
            MAT[II]:=SAVE[KK];
            II:=II+1;
          END;
      MAT[II]:=' ';
      II:=II+1;
      II:=II+1;
    END;
  MAT[II]:='*';
END;

```

```

PROCEDURE LOGSUM;
BEGIN
  I:=0;
  SUMAIO:=0.0;
  FOR KK:=1 TO NION DO
    BEGIN
      SUMAIO:=SUMAIO+COEF[KK+2]*LOG(AION[KK]);
    END;
  END;

PROCEDURE EQB1;
BEGIN
  MI:=MI+1;
  IONLIN[MI]:=0;
  IF (AM[M]<>1) OR (AM[A]<>1) THEN IONLIN[MI]:=2;
  IF (AM[M]<>1) AND (AM[A]<>1) THEN IONLIN[MI]:=1;
  IF MI=INDEX THEN
    BEGIN
      IF INDEX<>1 THEN DRAWER(79);
      INDEX:=INDEX+70;
      LNFD(15);
      WRITELN(CHR(12));
      DRAWER(79);
      WRITELN('');
      WRITE('NUMBER ! EQUILIBRIUM !');
      WRITELN(' BALANCED CHEMICAL EQUATION');
      WRITELN('');
      DRAWER(79);
    END;
  ACT1:=AM[M];
  ACT2:=AM[A];
  FOR HH:=1 TO 15 DO NAME[NION+3,HH]:=SP[A,HH];
  COEF[NION+3]:=METAL[M];
  COEF[1]:=METAL[A];
  FOR I:=1 TO NION DO
    COEF[I+2]:=COEF[NION+3]*ION[I,A]-COEF[1]*ION[I,M];
  SUMNUM;
  NUMB:=NION+5;
  FOR HH:=1 TO 15 DO TEMP[HH]:=NAME[1,HH];
  LINE[1,MI]:=M;
  LINE[2,MI]:=A;
  IF ((COEF[NION+3]=0) AND (COEF[NION+4](<0)) OR (COEF[NION+5](<0)) THEN
    UPDATE;
  END;

PROCEDURE EQBALANCER;
BEGIN
  MI:=0;
  NAME[2,1]:='H';
  NAME[2,2]:='2';
  NAME[2,3]:='O';
  NAME[NION+4,1]:='H';
  NAME[NION+4,2]:='+';
  NAME[NION+5,1]:='E';
  NAME[NION+5,2]:='-';
  NPP:=NP-1;
  FOR M:=1 TO NPP DO
    BEGIN
      FOR HH:=1 TO 15 DO NAME[1,HH]:=SP[M,HH];
      K:=M+1;
      FOR A:=K TO NP DO
        BEGIN
          EQB1;
          LOGSUM;
          FINDSIGN;
          EQB4;
          CALCEQEO;
        END;
      END;
    END;
  END;

```



```

PROCEDURE DIAGRAM;
BEGIN
  DRAWER(78);
  IONS:=0;
  NONION:=0;
  FOR I:=1 TO NP DO
    IF AM(I)=1 THEN NONION:=NONION+1
    ELSE IONS:=IONS+1;
  IF NONION=0 THEN
    BEGIN
      LNFD(10);
      WRITELN(FF,' ** NO SOLID SPECIES DIAGRAM **');
    END
  ELSE
    BEGIN
      IONDIG:=0;
      STABLE1;
    END;

  IF IONS<=1 THEN
    BEGIN
      LNFD(10);
      WRITELN(FF,' *** NO DISSOLVED SPECIES DIAGRAM ***');
    END
  ELSE
    BEGIN
      IONDIG:=1;
      STABLE1;
    END;
  END;
END;

PROCEDURE OUTMENU;
BEGIN
  WHILE (OPT1<>'T') AND (OPT1<>'P') DO
    BEGIN
      WRITELN(CHR(12));
      IF AB=FALSE
        THEN WRITELN('          DATA OUTPUT OPTIONS ')
        ELSE WRITELN('          EQUATION LISTING OPTIONS');
      LF(3);WRITELN('          P - PRINTER');
      LF(1);WRITELN('          T - TERMINAL');
      LF(2);WRITE('          ENTER OPTION:');
      READLN(OPT1);
      WRITELN(CHR(12));WRITELN;
    END;
  IF OPT1='P' THEN FILENAME:='PRINTER: '
  ELSE FILENAME:='CONSOLE: ';
END;

```

```

(*$N+*)
BEGIN
  REPEAT
    WRITELN(CHR(12));
    INITIALIZE;
    DATAINPUT;
    METALINPUT;
    WRITE(' MODIFY DATA ? [Y/N]: ');
    READLN(OPT1);
    IF OPT1='Y' THEN DATACORRECT;
    WRITELN(CHR(12));
    REPEAT
      IF NOPT='Y' THEN DATACORRECT;
      REPEAT
        LF(1);WRITE(' DISPLAY TABULATED DATA ? [Y/N]: ');
        READLN(OPT1);
        AB:=FALSE;
        IF OPT1='Y' THEN
          BEGIN
            OUTMENU;
            REWRITE(FFF,FILENAME);
            NONMETALDISPLAY;
            METALDISPLAY;
            CLOSE(FFF);
            OPT1:=' ';
            WHILE (OPT1<>'Y') AND (OPT1<>'N') DO
              BEGIN
                WRITE(' MODIFY DATA ? [Y/N]: ');
                READLN(OPT1);
              END;
            IF OPT1='Y' THEN DATACORRECT;
          END;
        AB:=TRUE;
        OUTMENU;
        REWRITE(FF,FILENAME);
        EQBALANCER;
        DIAGRAM;
        CLOSE(FF);
        LF(2);
        WRITELN(' EXECUTION COMPLETE....');
        LF(3);
        WRITE(' EXECUTE AGAIN ? [Y/N]: ');
        READLN(NOPT);
        IF NOPT='N' THEN EXIT(PROGRAM);
        INDEX:=1;
        WRITELN(CHR(12));
        LF(2);
        WRITE(' REPEAT WITH SAME DATA ? [Y/N]: ');
        READLN(NOPT);
      UNTIL NOPT='N';
      LF(2);
      WRITE(' MODIFY CURRENT DATA SET ? [Y/N]: ');
      READLN(NOPT);
    UNTIL NOPT='N';
  UNTIL NOPT='X';
END

```

(**S+*)

UNIT GETVALUE; INTRINSIC CODE 23 DATA 24;

INTERFACE

TYPE

AO15=ARRAY[1..15] OF CHAR;

AOI15=ARRAY[1..15] OF INTEGER;

PROCEDURE GETVAL(X:INTEGER;

VAR CCHAR:AO15);

IMPLEMENTATION

VAR HH,I : INTEGER;

INT :AOI15;

VAL :AOI15;

PROCEDURE GETVAL;

BEGIN

FOR I:=1 TO 15 DO

BEGIN

INT[I]:=0;

VAL[I]:=0;

CCHAR[I]:=' ';

END;

HH:=1;

WHILE X>= 1 DO

BEGIN

INT[HH]:=X;

X:=X DIV 10;

HH:=HH+1;

END;

VAL[HH]:=INT[HH];

FOR I:=1 TO (HH-1) DO

VAL[HH+1-I]:=INT[I]-10*INT[I+1];

FOR I:=1 TO HH DO

CCHAR[I]:=CHR(VAL[I]+ORD('0'));

FOR I:=1 TO (HH-1) DO

CCHAR[I]:=CCHAR[I+1];

CCHAR[HH]:=' ';

END;

BEGIN

END.

(*S*)

UNIT CONVERT. INTRINSIC CODE 16 DATA 17;

INTERFACE

TYPE
AOCH3=ARRAY[1..3] OF CHAR;
AOCH11=ARRAY[1..11] OF CHAR;

VAR
NUMBER : INTEGER;
CH3 : AOCH3;
ERROR : BOOLEAN;
CH11 : AOCH11;
RNUMBER: REAL;
PROCEDURE CHARTOINT;
PROCEDURE CHARTOREAL;

IMPLEMENTATION

VAR I : INTEGER;
BLANK: BOOLEAN;
POWER: REAL;

PROCEDURE CHARTOINT;
BEGIN

I:=3;
NUMBER:=0;
BLANK:=FALSE;
POWER:=1.0;
ERROR:=FALSE;
WHILE (CH3[I]=' ') AND (I>1) DO I:=I-1;
IF (I=1) AND (CH3[I]=' ') THEN

THEN
BEGIN
WRITELN;
WRITELN('NUMBER EXPECTED');
ERROR:=TRUE;

END

ELSE

BEGIN

WHILE (ERROR=FALSE) AND (I>0) AND (BLANK=FALSE) DO
IF CH3[I] IN ['0'..'9','-','] THEN

BEGIN

IF CH3[I]='-' THEN

NUMBER:=-NUMBER

ELSE NUMBER:=NUMBER+(ORD(CH3[I])-ORD('0'))*TRUNC(POWER)

POWER:=POWER*10.0;

I:=I-1;

END

ELSE

IF CH3[I]=' ' THEN

BLANK:=TRUE

ELSE

BEGIN

WRITELN;

WRITELN(' IMPROPER NUMBER');

ERROR:=TRUE;

END;

END;

END;

```

PROCEDURE CHARTOREAL.
BEGIN
    I:=1;
    RNUMBER:=0;
    BLANK:=FALSE;
    POWER:=1.0;
    ERROR:=FALSE;
    WHILE (CH1(I)=' ') AND (I>1) DO I:=I-1;
    IF (I=1) AND (CH1(I)=' ') THEN
        BEGIN
            WRITELN;
            WRITELN(' NUMBER EXPECTED');
            ERROR:=TRUE;
        END
    ELSE
        BEGIN
            WHILE (ERROR=FALSE) AND (I>0) AND (BLANK=FALSE) DO
                IF CH1(I) IN ['0','1','2','3','4','5','6','7','8','9'] THEN
                    IF CH1(I)='0' THEN
                        BEGIN
                            RNUMBER:=RNUMBER/POWER;
                            POWER:=1.0;
                            I:=I-1;
                        END
                    ELSE
                        BEGIN
                            IF CH1(I)='-' THEN
                                RNUMBER:=-RNUMBER
                            ELSE
                                BEGIN
                                    RNUMBER:=RNUMBER+(ORD(CH1(I))-ORD('0'))*POWER;
                                    POWER:=POWER*10.0;
                                END;
                                I:=I-1;
                            END
                        END
                    ELSE
                        IF CH1(I)=' ' THEN
                            BLANK:=TRUE
                        ELSE
                            BEGIN
                                WRITELN;
                                WRITELN(' IMPROPER NUMBER');
                                ERROR:=TRUE;
                            END;
                        END;
                END;
            END;
        END;
    END;
END;
BEGIN
END.

```

UNIT STABLE; INTRINSIC CODE 26 DATA 27;

INTERFACE

USES CONVERT, INDATA;

TYPE

AOINT2X595=ARRAY[1..2,1..595] OF INTEGER;

AOINT595 =ARRAY[1..595] OF INTEGER;

AOR2X595 =ARRAY[1..2,1..595] OF REAL;

VAR FF:TEXT;

FILENAME:STRING;

MI : INTEGER;

LINE :AOINT2X595;

LTYPE :AOINT595;

EQUAT :AOR2X595;

IONDIG : INTEGER;

IONLIN :AOINT595;

PROCEDURE STABLE1;

PROCEDURE LNFD(QQ:INTEGER);

PROCEDURE DRAWER(QQ:INTEGER);

IMPLEMENTATION

VAR

NUMB1,LINNO,LINNN,LTYPE1

:ARRAY[1..34] OF INTEGER;

I1,L1,L2,INDEX,JINDEX,I,N,NN,PASS

:INTEGER;

PHMIND,PHMAXD,K,JJ,HH,J

:INTEGER;

LINE1

:ARRAY[1..2,1..34] OF INTEGER;

EQUAT1

:ARRAY[1..2,1..34] OF REAL;

LOWER,UPPER

:ARRAY[1..4,1..34] OF REAL;

PHTEST

:ARRAY[1..35] OF REAL;

INTERC,EMINU,EMINL,PH1,PH2

:REAL;

ABC,POT1,POT2,POT11,POT22,E1,E2

:REAL;

PHMIN,PHMAX,EMAXU,EMAXL,PHINT

:REAL;

FLAG1,FLAG3,FLAG4,FLAG6,FLAGGER

:BOOLEAN;

FLAG5,FLAG7,FLAG8,FLAG9,FLAG10

:BOOLEAN;

PROCEDURE LNFD;

VAR Q:INTEGER;

BEGIN

FOR Q:=1 TO QQ DO WRITELN(FF);

END;

PROCEDURE DRAWER;

VAR Q:INTEGER;

BEGIN

FOR Q:=1 TO QQ DO WRITE(FF,'-');

WRITELN(FF);

END;

PROCEDURE RITER(ARG1,ARG2:REAL;

ARG3,ARG4:REAL;

ARG5:INTEGER);

BEGIN

WRITE(FF,' ',ARG1:7:3,' ',ARG2:6:2);

WRITE(FF,' ',ARG3:7:3,' ');

WRITELN(FF,ARG4:6:2,' ',ARG5:3,' ');

END;

PROCEDURE SUB1;

BEGIN

IF (POT11<POT1) AND (PHMIND<>0) THEN

RITER(POT1,UPPER[3,1],POT11,LOWER[3,1],NUMB1[PHMIND]);

IF (POT11<POT1) AND (PHMIND=0) THEN

BEGIN

WRITE(FF,' ',POT1:7:3,' ');

WRITE(FF,UPPER[3,1]:6:2,' ',POT11:7:3);

WRITELN(FF,' ',LOWER[3,1]:6:2,' ');

END;

IF (POT22<POT2) AND (PHMAXD<>0) THEN

RITER(POT2,UPPER[4,N],POT22,LOWER[4,NN],NUMB1[PHMAXD]);

IF (POT22<POT2) AND (PHMAXD=0) THEN

BEGIN

WRITE(FF,' ',POT2:7:3,' ');

WRITE(FF,UPPER[4,N]:6:2,' ',POT22:7:3);

WRITELN(FF,' ',LOWER[4,NN]:6:2,' ');

END;

END;

PROCEDURE STABLE11;

BEGIN

FOR I:=1 TO N DO

BEGIN

POT1:=UPPER[1,I]+UPPER[2,I]*UPPER[3,I];

POT2:=UPPER[1,I]+UPPER[2,I]*UPPER[4,I];

RITER(POT1,UPPER[3,I],POT2,UPPER[4,I],LINNO[I]);

END;

FOR I:=1 TO NN DO

BEGIN

POT1:=LOWER[1,I]+LOWER[2,I]*LOWER[3,I];

POT2:=LOWER[1,I]+LOWER[2,I]*LOWER[4,I];

RITER(POT1,LOWER[3,I],POT2,LOWER[4,I],LINNN[I]);

END;

POT1:=UPPER[1,I]+UPPER[2,I]*UPPER[3,I];

POT11:=LOWER[1,I]+LOWER[2,I]*LOWER[3,I];

POT11:=POT11+0.0001;

POT2:=UPPER[1,N]+UPPER[2,N]*UPPER[4,N];

POT22:=LOWER[1,NN]+LOWER[2,NN]*LOWER[4,NN];

POT22:=POT22+0.0001;

SUB1;

FLAGGER:=TRUE;

END;

PROCEDURE STABLE10;

BEGIN

LNFD(2);

WRITE(FF,' ');

DRAWER(57);

WRITE(FF,' ! POTENTIAL 1 ! PH 1 !');

WRITELN(FF,' POTENTIAL 2 ! PH 2 ! LINE NO. 1');

WRITE(FF,' ');

DRAWER(57);

END;

PROCEDURE STABLE9;

BEGIN

FLAG10:=FALSE;

IF EMAXL>EMAXU THEN

BEGIN

WHILE FLAG10=FALSE DO

BEGIN

IF (UPPER[4,N]>PHTEST[K])AND(N>1) THEN N:=N-1;

IF (LOWER[4,NN]>PHTEST[K])AND(NN>1) THEN NN:=NN-1;

K:=K-1;

EMAXL:=LOWER[1,NN]+LOWER[2,NN]*PHTEST[K];

EMAXU:=UPPER[1,N]+UPPER[2,N]*PHTEST[K];

IF EMAXU>EMAXL THEN FLAG10:=TRUE;

END;

PHINT:=(UPPER[1,N]-LOWER[1,NN])/(LOWER[2,NN]-UPPER[2,N]);

LOWER[4,NN]:=PHINT;

UPPER[4,N]:=PHINT;

END;

END;

PROCEDURE STABLE8;

BEGIN

IF FLAG8=FALSE THEN

BEGIN

PHINT:=(UPPER[1,1]-LOWER[1,1])/(LOWER[2,1]-UPPER[2,1]);

LOWER[3,1]:=PHINT;

UPPER[3,1]:=PHINT;

END;

END;

PROCEDURE SUB4(L:INTEGER);

BEGIN

LOWER[1,L]:=LOWER[1,L+1];

LOWER[2,L]:=LOWER[2,L+1];

LOWER[3,L]:=LOWER[3,L+1];

LOWER[4,L]:=LOWER[4,L+1];

LINNN[L]:=LINNN[L+1];

END;

PROCEDURE SUB5(L:INTEGER);

BEGIN

UPPER[1,L]:=UPPER[1,L+1];

UPPER[2,L]:=UPPER[2,L+1];

UPPER[3,L]:=UPPER[3,L+1];

UPPER[4,L]:=UPPER[4,L+1];

LINNO[L]:=LINNO[L+1];

END;

```

PROCEDURE STABLE7;
VAR L: INTEGER;
BEGIN
  FLAG8:=FALSE;
  IF EMINL<EMINU THEN FLAG8:=TRUE;
  IF FLAG8=FALSE THEN
    BEGIN
      I:=1;
      FLAG9:=FALSE;
      WHILE FLAG9=FALSE DO
        BEGIN
          I:=I+1;
          ABC:=PHTEST(I);
          IF (ABC<0.000000001) AND (ABC>-0.000000001) THEN ABC:=0.0;
          EMINL:=LOWER(1,I)+LOWER(2,I)*ABC;
          EMINU:=UPPER(1,I)+UPPER(2,I)*ABC;
          IF (EMINU<EMINL) AND (I=K) THEN FLAG7:=TRUE;
          IF (FLAG7=FALSE) THEN
            IF EMINL<EMINU THEN FLAG9:=TRUE;
            IF (FLAG7=FALSE) AND (FLAG9=FALSE) THEN
              BEGIN
                IF LOWER(4,I)<=PHTEST(I) THEN LINNN(I):=0;
                IF UPPER(4,I)<=PHTEST(I) THEN LINNO(I):=0;
                IF LINNN(I)=0 THEN
                  BEGIN
                    NN:=NN-1;
                    FOR L:=1 TO NN DO SUB4(L);
                  END;
                IF LINNO(I)=0 THEN
                  BEGIN
                    N:=N-1;
                    FOR L:=1 TO N DO SUB5(L);
                  END;
                END;
              END;
            IF I=35 THEN FLAG9:=TRUE;
          END;
        END;
      END;
END;

PROCEDURE SUB3;
BEGIN
  PHTEST(K):=UPPER(4,I);
  IF (I=N) AND (JJ=NN) THEN FLAG6:=TRUE;
  IF FLAG6=FALSE THEN
    BEGIN
      IF I<N THEN I:=I+1;
      IF JJ<NN THEN JJ:=JJ+1;
      K:=K+1;
    END;
  END;
END;

PROCEDURE STABLE6;
BEGIN
  IF FLAG5=FALSE THEN
    BEGIN
      I:=1;
      JJ:=1;
      K:=2;
      PHTEST(I):=PHMIN;
      FLAG6:=FALSE;
      WHILE FLAG6=FALSE DO
        BEGIN
          IF UPPER(4,I)<LOWER(4,JJ) THEN
            BEGIN
              PHTEST(K):=UPPER(4,I);
              K:=K+1;
              I:=I+1;
            END
          ELSE
            IF LOWER(4,JJ)<UPPER(4,I) THEN
              BEGIN
                PHTEST(K):=LOWER(4,JJ);
                K:=K+1;
                JJ:=JJ+1;
              END
            ELSE
              IF UPPER(4,I)=LOWER(4,JJ) THEN SUB3;
            END;
          END;
        END;
      END;
    END;
  END;
END;

```



```

PROCEDURE STABLE5;
BEGIN
  EMINL:=LOWER(1,1)+LOWER(2,1)*PHMIN;
  EMINU:=UPPER(1,1)+UPPER(2,1)*PHMIN;
  EMAXL:=LOWER(1,NN)+LOWER(2,NN)*PHMAX;
  EMAXU:=UPPER(1,N)+UPPER(2,N)*PHMAX;
  IF (EMINL<EMINU) AND (EMAXL<EMAXU) THEN FLAG5:=TRUE;
END;

PROCEDURE SUB8;
BEGIN
  LNFD(2);
  WRITE(FF, ' ');
  DRAWER(55);
  WRITE(FF, ' ');
  WRITELN(FF, ' POTENTIAL 2 ! PH 2 ! LINE NO. !');
  WRITE(FF, ' ');
  DRAWER(55);
  IF N<>0 THEN
    FOR I:=1 TO N DO
      BEGIN
        POT1:=UPPER(1,I)+UPPER(2,I)*UPPER(3,I);
        POT2:=UPPER(1,I)+UPPER(2,I)*UPPER(4,I);
        RITER(POT1,UPPER(3,I),POT2,UPPER(4,I),LINNO(I));
      END
    ELSE
      FOR I:=1 TO NN DO
        BEGIN
          POT1:=LOWER(1,I)+LOWER(2,I)*LOWER(3,I);
          POT2:=LOWER(1,I)+LOWER(2,I)*LOWER(4,I);
          RITER(POT1,LOWER(3,I),POT2,LOWER(4,I),LINNN(I));
        END
      END;

END;

PROCEDURE INTERIMWRITER;
BEGIN
  IF (N=0) OR (NN=0) THEN
    BEGIN
      IF N=0 THEN
        BEGIN
          LNFD(2);
          WRITELN(FF, ' NO UPPER LIMIT');
        END;
      IF NN=0 THEN
        BEGIN
          LNFD(2);
          WRITELN(FF, ' NO LOWER LIMIT');
        END;
      IF (N<>0) OR (NN<>0) THEN
        SUB8;
      IF PHMIN<-2.0 THEN
        BEGIN
          LNFD(1);
          WRITE(FF, ' ');
          WRITE(FF, 'MINIMUM PH = ', PHMIN:6:2, ' LINE NO. ');
          WRITELN(FF, NUMB1[PHMIND]:4);
        END;
      IF PHMIN<=-2.0 THEN
        WRITELN(FF, ' MINIMUM PH = ', PHMIN:6:2);
      IF PHMAX<16.0 THEN
        BEGIN
          WRITE(FF, ' MAXIMUM PH = ', PHMAX:6:2);
          WRITELN(FF, 'PHMAXD= ', PHMAXD:4);
          WRITELN(FF, ' LINE NO. ', NUMB1[PHMAXD]:4);
        END;
      IF PHMAX<=16.0 THEN
        WRITELN(FF, ' MAXIMUM PH = ', PHMAX:6:2);
      FLAGGER:=TRUE;
    END;
END;

```

```

PROCEDURE TEMP2;
BEGIN
  FLAG3:=FALSE;
  NN:=NN+1;
  LOWER[1,NN]:=EQUAT1[1,L1];
  LOWER[2,NN]:=EQUAT1[2,L1];
  LOWER[3,NN]:=PH1;
  LINNN[NN]:=NUMB1[L1];
  LOWER[4,NN]:=PHMAX;
  IF PASS<1 THEN FLAG3:=TRUE;
  IF FLAG3=FALSE THEN
    BEGIN
      LOWER[4,NN]:=PH2;
      IF PH2>PHMAX THEN LOWER[4,NN]:=PHMAX;
      IF PH2=PHMAX THEN FLAG3:=TRUE;
      IF FLAG3=FALSE THEN
        BEGIN
          PH1:=PH2;
          E1:=EQUAT1[1,L2]+EQUAT1[2,L2]*PH1;
          L1:=L2;
        END;
      END;
    END;
END;

PROCEDURE TEMP1;
BEGIN
  FLAG1:=FALSE;
  N:=N+1;
  UPPER[1,N]:=EQUAT1[1,L1];
  UPPER[2,N]:=EQUAT1[2,L1];
  UPPER[3,N]:=PH1;
  LINNO[N]:=NUMB1[L1];
  UPPER[4,N]:=PHMAX;
  IF PASS<1 THEN FLAG1:=TRUE;
  IF FLAG1=FALSE THEN
    BEGIN
      UPPER[4,N]:=PH2;
      IF PH2>PHMAX THEN UPPER[4,N]:=PHMAX;
      IF PH2=PHMAX THEN FLAG1:=TRUE;
      IF FLAG1=FALSE THEN
        BEGIN
          PH1:=PH2;
          E1:=EQUAT1[1,L2]+EQUAT1[2,L2]*PH1;
          L1:=L2;
        END;
      END;
    END;
END;

PROCEDURE LOWBNDLNS;
BEGIN
  FOR I:=1 TO I1 DO
    IF (LINE1[2,I]=J) AND (LTYPE1[I]=2) THEN
      BEGIN
        PASS:=PASS+1;
        IF PASS=1 THEN
          BEGIN
            E1:=EQUAT1[1,I]+EQUAT1[2,I]*PH1;
            L1:=I;
          END
        ELSE
          BEGIN
            E2:=EQUAT1[1,I]+EQUAT1[2,I]*PH1;
            IF E2>E1 THEN
              BEGIN
                E1:=E2;
                L1:=I;
              END;
            END;
          END;
        END;
      END;
END;
END;

```

```

PROCEDURE INTPTSLO;
BEGIN
  PASS:=0;
  FOR I:=1 TO I1 DO
    BEGIN
      IF (LINE1[2,I]=J) AND (LTYPE1[I]=2) AND
        (EQUAT1[2,I]EQUAT1[2,L1]) THEN
        BEGIN
          PASS:=PASS+1;
          IF PASS<= 1 THEN
            BEGIN
              PH2:=EQUAT1[1,L1]-EQUAT1[1,I];
              PH2:=PH2/(EQUAT1[2,I]-EQUAT1[2,L1]);
              L2:=I;
            END
          ELSE
            BEGIN
              INTERC:=EQUAT1[1,L1]-EQUAT1[1,I];
              INTERC:=INTERC/(EQUAT1[2,I]-EQUAT1[2,L1]);
              IF (INTERC<=PH2) AND (INTERC>=PH1) THEN
                BEGIN
                  L2:=I;
                  PH2:=INTERC
                END;
            END;
          END;
        END;
      END;
    END;
  END;
  TEMP2;
END;

```

```

PROCEDURE INTPTSH1;
BEGIN
  PASS:=0;
  FOR I:=1 TO I1 DO
    IF (LINE1[1,I]=J) AND (LTYPE1[I]=2) THEN
      IF EQUAT1[2,I]EQUAT1[2,L1] THEN
        BEGIN
          PASS:=PASS+1;
          IF PASS<=1 THEN
            BEGIN
              PH2:=EQUAT1[1,L1]-EQUAT1[1,I];
              PH2:=PH2/(EQUAT1[2,I]-EQUAT1[2,L1]);
              L2:=I;
            END
          ELSE
            BEGIN
              INTERC:=EQUAT1[1,L1]-EQUAT1[1,I];
              INTERC:=INTERC/(EQUAT1[2,I]-EQUAT1[2,L1]);
              IF INTERC<=PH2 THEN
                BEGIN
                  L2:=I;
                  PH2:=INTERC;
                END;
              END;
            END;
          END;
        END;
      END;
    END;
  END;
  TEMP1;
END;

```

```

PROCEDURE UPBNDLNS;
BEGIN
  PASS:=0;
  FOR I:=1 TO I1 DO
    IF (LINE1[1,I]=J) AND (LTYPE1[I]=2) THEN
      BEGIN
        PASS:=PASS+1;
        IF PASS=1 THEN
          BEGIN
            E1:=EQUAT1[1,I]+EQUAT1[2,I]*PH1;
            L1:=I;
          END
        ELSE
          BEGIN
            E2:=EQUAT1[1,I]+EQUAT1[2,I]*PH1;
            IF E2<=E1 THEN
              BEGIN
                E1:=E2;
                L1:=I;
              END;
            END;
          END;
        END;
      END;
    END;
  END;
  END;
END;

```

```

PROCEDURE STABLE4;
BEGIN
  PHMAX:=16.0;
  PHMAXD:=0;
  FOR I:=1 TO I1 DO
    IF LINE1[1,I]=J THEN
      IF LTYPE1[I]=1 THEN
        IF EQUAT1[1,I]<PHMAX THEN
          BEGIN
            PHMAX:=EQUAT1[1,I];
            PHMAXD:=I;
          END;
        END;
      END;
  END;

PROCEDURE STABLE3;
BEGIN
  PHMIN:=-2.0;
  PHMIND:=0;
  FOR I:=1 TO I1 DO
    IF (LINE1[2,I]=J) THEN
      IF (LTYPE1[I]=1) THEN
        IF (EQUAT1[1,I]>PHMIN) THEN
          BEGIN
            PHMIN:=EQUAT1[1,I];
            PHMIND:=I;
          END;
        END;
      END;
  END;

PROCEDURE STABLE2;
BEGIN
  I1:=I1+1;
  LINE1[1,I1]:=LINEC1[I];
  LINE1[2,I1]:=LINEC2[I];
  LTYPE1[I1]:=LTYPEC[I];
  EQUAT1[1,I1]:=EQUATC1[I];
  EQUAT1[2,I1]:=EQUATC2[I];
  NUMB1[I1]:=1;
END;

PROCEDURE START;
BEGIN
  INDEX:=1;
  JINDEX:=0;
END;

PROCEDURE SETFLAGS;
BEGIN
  FLAGGER:=FALSE;
  FLAG1:=FALSE; FLAG3:=FALSE;
  FLAG4:=FALSE; FLAG5:=FALSE;
  FLAG6:=FALSE; FLAG7:=FALSE;
  FLAG8:=FALSE; FLAG9:=FALSE;
  FLAG10:=FALSE;
END;

```

```

PROCEDURE STABLE1;
BEGIN
  START;
  FOR J:=1 TO NP DO
  BEGIN
    SETFLAGS;
    IF (IONDIG<>1) OR (AM[J]<>1.0) THEN
    BEGIN
      JINDEX:=JINDEX+1;
      N:=0;
      NN:=0;
      I1:=0;
      IF JINDEX=INDEX THEN WRITELN(CHR(12));
      IF JINDEX=INDEX THEN INDEX:=INDEX+5;
      LNFD(4);
      WRITELN(FF,'*****');
      WRITE(FF,'*   AREA OF PREDOMINANCE FOR: ');
      FOR HH:=1 TO 15 DO WRITE(FF,SPIJ,HH);
      WRITE(FF,' *');
      IF IONDIG=1 THEN WRITE(FF,' DISSOLVED SPECIES DIAGRAM');
      LNFD(1);
      WRITELN(FF,'*****');
      FOR I:=1 TO MI DO
      IF (LINE[I,I]=J) OR (LINE[2,I]=J) THEN
      IF (IONDIG<>1) OR (IONLIN[I]=1) THEN
      STABLE2;
      STABLE3;
      IF PHMIN<16 THEN
      BEGIN
        STABLE4;
        IF PHMAX>= PHMIN THEN
        BEGIN
          PH1:=PHMIN;
          PH2:=PHMAX;
          UPBNDLNS;
          IF PASS=0 THEN FLAG1:=TRUE;
          IF FLAG1=FALSE THEN
          BEGIN
            IF PASS=1 THEN TEMP1;
            WHILE FLAG1=FALSE DO INTPTSHI;
          END;
          PH1:=PHMIN;
          PH2:=PHMAX;
          PASS:=0;
          LOWBNDLNS;
          IF PASS=0 THEN FLAG3:=TRUE;
          IF FLAG3=FALSE THEN
          BEGIN
            IF PASS=1 THEN TEMP2;
            WHILE FLAG3=FALSE DO INTPTSLO;
          END;
          INTERIMWRITER;
          IF FLAGGER=FALSE THEN
          BEGIN
            STABLE5;
            STABLE6;
            IF FLAG5=FALSE THEN STABLE7;
            IF (FLAG7=FALSE) AND (FLAG5=FALSE) THEN STABLE8;
            IF (FLAG7=FALSE) AND (FLAG5=FALSE) THEN STABLE9;
            IF FLAG7=FALSE THEN STABLE10;
            IF FLAG7=FALSE THEN STABLE11;
          END;
        END;
      END;
      IF FLAGGER=FALSE THEN
      BEGIN
        LNFD(4);
        WRITE(FF,' NO AREA OF PREDOMINANCE');
        LNFD(2);
      END;
    END;
  END;
END;
LNFD(4);
END;
BEGIN
END.

```

(**S+*)

UNIT INDATA; INTRINSIC CODE 18 DATA 19;

INTERFACE

USES CONVERT;

TYPE

AON=ARRAY[1..15,1..15] OF CHAR;
ASP=ARRAY[1..35,1..15] OF CHAR;
AO10=ARRAY[1..10] OF REAL;
AINT10=ARRAY[1..10] OF INTEGER;
A35=ARRAY[1..35] OF REAL;
AI35=ARRAY[1..35] OF INTEGER;
M10X35=ARRAY[1..10] OF AI35;

VAR

NAME : AON;
SP : ASP;
T : REAL;
FEH2O : REAL;
NION : INTEGER;
FION : AO10;
AION : AO10;
ZION : AINT10;
BION : AINT10;
OXY : AINT10;
HYD : AINT10;
NP : INTEGER;
AM,F : A35;
Z : AI35;
METAL : AI35;
OXYGEN : AI35;
HYDRO : AI35;
ION : M10X35;
FFF : TEXT;

PROCEDURE GETNONMET;
PROCEDURE GETMET;
PROCEDURE DATAINPUT;
PROCEDURE METALINPUT;
PROCEDURE DATACORRECT;
PROCEDURE IONSOUT1;
PROCEDURE IONSOUT2;
PROCEDURE NONMETALDISPLAY;
PROCEDURE DIS1MET;
PROCEDURE METALDISPLAY;
PROCEDURE LF(QQ: INTEGER);
PROCEDURE INCHAR;
PROCEDURE INREAL;

IMPLEMENTATION

VAR I: INTEGER;
Q,M: INTEGER;
L: INTEGER;
KK,J: INTEGER;
K: INTEGER;
HH: INTEGER;
XYX: INTEGER;

PROCEDURE LF;

BEGIN
FOR L:=1 TO QQ DO WRITELN;
END;

PROCEDURE DRAW(QQ: INTEGER);

BEGIN
FOR L:=1 TO QQ DO WRITE(FFF,'-');
WRITELN(FFF);
END;

```

PROCEDURE INCHAR;
BEGIN
  FOR HH:=1 TO 3 DO CH3[HH]:=' ';
  HH:=1;
  WHILE (NOT EOLN) AND (HH<4) DO
  BEGIN
    READ(CH3[HH]);
    IF CH3[HH]=CHR(8) THEN
    BEGIN
      WRITE(CHR(8));
      HH:=HH-2;
    END;
    HH:=HH+1;
  END;
  READLN;
  CHARTOINT;
END;

```

```

PROCEDURE INREAL;
BEGIN
  FOR HH:=1 TO 11 DO CH11[HH]:=' ';
  HH:=1;
  WHILE (NOT EOLN) AND (HH<12) DO
  BEGIN
    READ(CH11[HH]);
    IF CH11[HH]=CHR(8) THEN
    BEGIN
      WRITE(CHR(8));
      HH:=HH-2;
    END;
    HH:=HH+1;
  END;
  READLN;
  CHARTOREAL;
END;

```

```

PROCEDURE GETNONMET;
BEGIN
  HH:=1;
  WHILE NOT EOLN DO
  BEGIN
    READ(NAME[K,HH]);
    IF NAME[K,HH]=CHR(8) THEN
    BEGIN
      WRITE(CHR(8));
      HH:=HH-2;
    END;
    HH:=HH+1;
  END;
  READLN;
END;

```

```

PROCEDURE GETMET;
BEGIN
  HH:=1;
  WHILE NOT EOLN DO
  BEGIN
    READ(SP[M,HH]);
    IF SP[M,HH]=CHR(8) THEN
    BEGIN
      WRITE(CHR(8));
      HH:=HH-2;
    END;
    HH:=HH+1;
  END;
  READLN;
END;

```

```

PROCEDURE DATAINPUT;
BEGIN
  ERROR:=TRUE;
  WHILE ERROR=TRUE DO
    BEGIN
      LF(1);WRITE(' ENTER TEMPERATURE (IN DEGREES KELVIN): ');
      INREAL;
    END;
    T:=RNUMBER;
    ERROR:=TRUE;
    WHILE ERROR=TRUE DO
      BEGIN
        LF(1);WRITE(' ENTER GIBBS FREE ENERGY OF FORMATION');
        LF(1);WRITE(' OF WATER AT ',T:4:2,' DEGREES (CALS/MOLE): ');
        INREAL;
      END;
      FEH2O:=RNUMBER;
      ERROR:=TRUE;
      WHILE ERROR=TRUE DO
        BEGIN
          LF(1);WRITE(' ENTER THE NUMBER OF NON-METALLIC SPECIES: ');
          INCHAR;
        END;
        NION:=NUMBER;
        IF NION <> 0 THEN
          BEGIN
            FOR I:=1 TO NION DO
              BEGIN
                K:=I+2;
                LF(1);WRITE(' NAME OF NON-METALLIC SPECIE # ',I:2,' ');
                GETNONMET;
                ERROR:=TRUE;
                WHILE ERROR=TRUE DO
                  BEGIN
                    LF(1);WRITE(' FREE ENERGY OF FORMATION: ');
                    INREAL;
                  END;
                  FION(I):=RNUMBER;
                  ERROR:=TRUE;
                  WHILE ERROR=TRUE DO
                    BEGIN
                      LF(1);WRITE(' IONIC ACTIVITY: ');
                      INREAL;
                    END;
                    AION(I):=RNUMBER;
                    ERROR:=TRUE;
                    WHILE ERROR=TRUE DO
                      BEGIN
                        LF(1);WRITE(' ELECTRICAL CHARGE: ');
                        INCHAR;
                      END;
                      ZION(I):=NUMBER;
                      ERROR:=TRUE;
                      WHILE ERROR=TRUE DO
                        BEGIN
                          LF(1);WRITE(' NUMBER OF CHARACTERISTIC ATOMS: ');
                          INCHAR;
                        END;
                        BION(I):=NUMBER;
                        ERROR:=TRUE;
                        WHILE ERROR=TRUE DO
                          BEGIN
                            LF(1);WRITE(' NUMBER OF OXYGEN ATOMS: ');
                            INCHAR;
                          END;
                          OXY(I):=NUMBER;
                          ERROR:=TRUE;
                          WHILE ERROR=TRUE DO
                            BEGIN
                              LF(1);WRITE(' NUMBER OF HYDROGEN ATOMS: ');
                              INCHAR;
                            END;
                            HYD(I):=NUMBER;
                            LF(1);
                            WRITELN(CHR(12));
                          END;
                        END;
                      END;
                    END;
                  END;
                END;
              END;
            END;
          END;
        END;
      END;
    END;
  END;
END;

```



```

PROCEDURE METALINPUT;
BEGIN
  WRITELN(CHR(12));
  ERROR:=TRUE;
  WHILE ERROR=TRUE DO
    BEGIN
      LF(1);WRITE('  ENTER NUMBER OF METALLIC SPECIES: ');
      INCHAR;
    END;
  NP:=NUMBER;
  FOR M:=1 TO NP DO
    BEGIN
      LF(1);WRITE('  NAME OF METALLIC SPECIE # ',M:2,' ');
      GETMET;
      ERROR:=TRUE;
      WHILE ERROR=TRUE DO
        BEGIN
          LF(1);WRITE('  FREE ENERGY OF FORMATION: ');
          INREAL;
        END;
      F(M):=RNUMBER;
      ERROR:=TRUE;
      WHILE ERROR=TRUE DO
        BEGIN
          LF(1);WRITE('  IONIC ACTIVITY: ');
          INREAL;
        END;
      AM(M):=RNUMBER;
      ERROR:=TRUE;
      WHILE ERROR=TRUE DO
        BEGIN
          LF(1);WRITE('  ELECTRICAL CHARGE: ');
          INCHAR;
        END;
      Z(M):=NUMBER;
      ERROR:=TRUE;
      WHILE ERROR=TRUE DO
        BEGIN
          LF(1);WRITE('  NUMBER OF METAL ATOMS: ');
          INCHAR;
        END;
      METAL(M):=NUMBER;
      ERROR:=TRUE;
      WHILE ERROR=TRUE DO
        BEGIN
          LF(1);WRITE('  NUMBER OF OXYGEN ATOMS: ');
          INCHAR;
        END;
      OXYGEN(M):=NUMBER;
      ERROR:=TRUE;
      WHILE ERROR=TRUE DO
        BEGIN
          LF(1);WRITE('  NUMBER OF HYDROGEN ATOMS: ');
          INCHAR;
        END;
      HYDRO(M):=NUMBER;
      IF NION > 0 THEN
        BEGIN
          FOR I:=1 TO NION DO
            BEGIN
              ERROR:=TRUE;
              WHILE ERROR=TRUE DO
                BEGIN
                  LF(1);
                  WRITELN('  ENTER NUMBER OF CHARACTERISTIC ATOMS');
                  WRITE('  FOR IONIC SPECIES # ',I:2,' ');
                  INCHAR;
                END;
              ION(I,M):=NUMBER;
            END;
          END;
        ELSE ION(1,M):=0;
      LF(1);
      WRITELN(CHR(12));
    END;
  END;
END;

```

```

PROCEDURE IONSOUT1;
BEGIN
  WRITE(FFF, ' ', I:2, ' ');
  FOR HH:=1 TO 8 DO WRITE(FFF, NAME[I+2, HH]);
  WRITE(FFF, ' ', FION[I:10:1, ' ']);
  WRITELN(FFF, AION[I:2:6, ' ', ZION[I:4, ' ']);
END;

PROCEDURE IONSOUT2;
BEGIN
  WRITE(FFF, ' ', I:2, ' ', BION[I:3, ' ']);
  WRITELN(FFF, ' ', OXY[I:2, ' ', HYD[I:2, ' ']);
END;

PROCEDURE NONMETALDISPLAY;
BEGIN
  WRITELN(CHR(12));
  WRITELN(FFF);
  WRITELN(FFF, '*****:39);
  WRITE(FFF, ' TEMPERATURE = ':29, T:5:2, '*');
  WRITELN(FFF, '*****:39);
  WRITELN(FFF);
  IF NION=0 THEN
    BEGIN
      WRITELN(FFF); WRITELN(FFF);
      WRITE(FFF, '*** NO NON-METALLIC IONIC SPECIES ');
      WRITE(FFF, 'ARE CONSIDERED ***');
      NION:=1;
    END
  ELSE
    BEGIN
      WRITELN(FFF);
      DRAW(53);
      WRITE(FFF, ' ION ! IONIC ! FREE ENERGY ');
      WRITELN(FFF, ' IONIC ! ');
      WRITE(FFF, 'NUMBER ! SPECIES ! OF FORMATION ');
      WRITELN(FFF, ' ACTIVITY ! CHARGE ! ');
      DRAW(53);
      FOR I:=1 TO NION DO
        IONSOUT1;
      FOR I:=1 TO 3 DO WRITELN(FFF);
      DRAW(45);
      WRITELN(FFF, ' ION ! CHARACTERISTIC ! OXYGEN ! HYDROGEN ! ');
      WRITELN(FFF, 'NUMBER ! ATOMS ! ATOMS ! ATOMS ! ');
      DRAW(45);
      FOR I:=1 TO NION DO
        IONSOUT2;
    END;
  END;

PROCEDURE DIS1MET;
BEGIN
  WRITE(FFF, ' ');
  FOR HH:=1 TO 15 DO WRITE(FFF, SP[I, HH]);
  WRITE(FFF, ' ', METAL[I:2, ' ', OXYGEN[I:2]);
  WRITE(FFF, ' ', HYDRO[I:2, ' ']);
  WRITELN(FFF);
END;

PROCEDURE DIS2MET;
BEGIN
  WRITE(FFF, ' ');
  FOR HH:=1 TO 15 DO WRITE(FFF, SP[I, HH]);
  WRITE(FFF, ' ');
  IF Q=1 THEN
    FOR J:=1 TO 5 DO
      IF J<=NION THEN
        WRITE(FFF, ' ', ION[J, I:2, ' ']);
  IF Q=2 THEN
    FOR J:=6 TO 10 DO
      IF J<=NION THEN
        WRITE(FFF, ' ', ION[J, I:2, ' ']);
  IF Q=3 THEN
    FOR J:=11 TO 15 DO
      IF J<=NION THEN
        WRITE(FFF, ' ', ION[J, I:2, ' ']);
  IF Q=4 THEN
    FOR J:=16 TO 20 DO
      IF J<=NION THEN
        WRITE(FFF, ' ', ION[J, I:2, ' ']);
  WRITELN(FFF);
END;

```

PROCEDURE DIS3MET;

```

BEGIN
  WRITE(FFF, ' ');
  IF Q=1 THEN
    WRITE(FFF, ' ION1 ION2 ION3 ION4 ION5 ');
  IF Q=2 THEN
    WRITE(FFF, ' ION6 ION7 ION8 ION9 ION10 ');
  IF Q=3 THEN
    WRITE(FFF, ' ION11 ION12 ION13 ION14 ION15 ');
  IF Q=4 THEN
    WRITE(FFF, ' ION16 ION17 ION18 ION19 ION20 ');
  WRITELN(FFF);
  DRAW(53);
END;
```

PROCEDURE METALDISPLAY;

```

BEGIN
  WRITELN(CHR(12));
  WRITELN(FFF);WRITELN(FFF);
  DRAW(53);
  WRITELN(FFF, '          ! FREE ENERGY ! SPECIES ! ');
  WRITELN(FFF, 'METALLIC SPECIES ! OF FORMATION ! ACTIVITY ! CHARGE !');
  DRAW(53);
  FOR I:=1 TO NP DO
    BEGIN
      WRITE(FFF, ' ');
      FOR HH:=1 TO 15 DO WRITE(FFF,SP(I,HH));
      WRITE(FFF, ' ',FC(I):11:1, ' ',AM(I):2:6);
      WRITELN(FFF, ' ',Z(I):2, ' ');
    END;
  FOR I:=1 TO 3 DO WRITELN(FFF);
  DRAW(46);
  WRITELN(FFF, '          ! METAL ! OXYGEN ! HYDROGEN !');
  WRITELN(FFF, 'METALLIC SPECIES ! ATOMS ! ATOMS ! ATOMS !');
  DRAW(46);
  FOR I:=1 TO NP DO DIS1MET;
  FOR I:=1 TO 3 DO WRITELN(FFF);
  L:=TRUNC((NION-1)/5.0)+1;
  FOR Q:=1 TO L DO
    BEGIN
      WRITELN(FFF);
      DRAW(53);
      WRITE(FFF, ' ');
      WRITELN(FFF, '          ! NUMBER OF CHARACTERISTIC ATOMS !');
      WRITE(FFF, 'METALLIC SPECIES !          OF EACH IONIC SPECIES');
      WRITELN(FFF, ' ');
      DIS3MET;
      FOR I:=1 TO NP DO DIS2MET;
      FOR I:=1 TO 3 DO WRITELN(FFF);
    END;
  END;
END;
```

PROCEDURE NMETC7;

```

BEGIN
  WRITE('          MODIFICATION OF NUMBER OF HYDROGEN ATOMS FOR ');
  FOR K:=1 TO 15 DO WRITE(NAME(KK,K));
  LF(3);
  WRITELN(' CURRENT VALUE IS ',HYD(I):3);
  ERROR:=TRUE;
  WHILE ERROR=TRUE DO
    BEGIN
      LF(1);
      WRITE(' DESIRED VALUE: ');
      INCHAR;
    END;
  HYD(I):=NUMBER;
END;
```

```

PROCEDURE NMETC6;
BEGIN
  WRITE('      MODIFICATION OF NUMBER OF OXYGEN ATOMS FOR ');
  FOR K:=1 TO 15 DO WRITE(NAME[KK,K]);
  LF(3);
  WRITELN(' CURRENT VALUE IS ',OXY[I]:3);
  ERROR:=TRUE;
  WHILE ERROR=TRUE DO
    BEGIN
      LF(1);
      WRITE(' DESIRED VALUE: ');
      INCHAR;
    END;
    OXY[I]:=NUMBER;
  END;
END;

PROCEDURE NMETC5;
BEGIN
  WRITE('      MODIFICATION OF NUMBER OF CHARACTERISTIC ATOMS');
  FOR K:=1 TO 15 DO WRITE(NAME[KK,K]);
  LF(3);
  WRITELN(' CURRENT VALUE IS ',BION[I]:3);
  ERROR:=TRUE;
  WHILE ERROR=TRUE DO
    BEGIN
      LF(1);
      WRITE(' DESIRED VALUE: ');
      INCHAR;
    END;
    BION[I]:=NUMBER;
  END;
END;

PROCEDURE NMETC4;
BEGIN
  WRITE('      MODIFICATION OF CHARGE FOR ');
  FOR K:=1 TO 15 DO WRITE(NAME[KK,K]);
  LF(3);
  WRITELN(' CURRENT VALUE IS ',ZION[I]:4);
  ERROR:=TRUE;
  WHILE ERROR=TRUE DO
    BEGIN
      LF(1);
      WRITE(' DESIRED VALUE: ');
      INCHAR;
    END;
    ZION[I]:=NUMBER;
  END;
END;

PROCEDURE NMETC3;
BEGIN
  WRITE('      MODIFICATION OF IONIC ACTIVITY FOR ');
  FOR K:=1 TO 15 DO WRITE(NAME[KK,K]);
  LF(3);
  WRITELN(' CURRENT VALUE IS ',AION[I]:2:6);
  ERROR:=TRUE;
  WHILE ERROR=TRUE DO
    BEGIN
      LF(1);
      WRITE(' DESIRED VALUE: ');
      INREAL;
    END;
    AION[I]:=RNUMBER;
  END;
END;

PROCEDURE NMETC2;
BEGIN
  WRITE('      MODIFICATION OF FREE ENERGY FOR ');
  FOR K:=1 TO 15 DO WRITE(NAME[KK,K]);
  LF(3);
  WRITELN(' CURRENT VALUE IS ',FION[I]:10:2);
  ERROR:=TRUE;
  WHILE ERROR=TRUE DO
    BEGIN
      LF(1);
      WRITE(' DESIRED VALUE: ');
      INREAL;
    END;
    FION[I]:=RNUMBER;
  END;
END;

```

```

PROCEDURE NMETC1;
BEGIN
  WRITELN('      MODIFICATION OF SPECIES NAME');
  LF(2);
  WRITE(' CURRENT NAME IS ');
  FOR K:=1 TO 15 DO WRITE(NAME(KK,K));
  LF(2);
  WRITE(' DESIRED NAME: ');
  FOR K:=1 TO 15 DO NAME[I,K]:=' ';
  K:=KK;
  GETNONMET;
END;

PROCEDURE NONMETCOR;
VAR FLAG2:BOOLEAN;
BEGIN
  WRITELN(CHR(12));
  WRITELN('      MODIFICATION OF NON-METALLIC SPECIES DATA');
  ERROR:=TRUE;
  WHILE ERROR=TRUE DO
    BEGIN
      LF(3);
      WRITE(' ENTER IONIC SPECIE NUMBER: ');
      INCHAR;
      IF (NUMBER<1) OR (NUMBER>NION) THEN ERROR:=TRUE;
    END;
    I:=NUMBER;
    KK:=I+2;
    REPEAT
      FLAG2:=FALSE;
      LF(2);
      WRITELN(' PARAMETER TO BE MODIFIED - ');
      LF(1);
      WRITELN('      1 - ION NAME');
      WRITELN('      2 - FREE ENERGY OF FORMATION');
      WRITELN('      3 - ACTIVITY');
      WRITELN('      4 - CHARGE');
      WRITELN('      5 - NUMBER OF CHARACTERISTIC ATOMS');
      WRITELN('      6 - NUMBER OF OXYGEN ATOMS');
      WRITELN('      7 - NUMBER OF HYDROGEN ATOMS');
      ERROR:=TRUE;
      WHILE ERROR=TRUE DO
        BEGIN
          LF(1);
          WRITE(' ENTER OPTION: ');
          INCHAR;
        END;
        J:=NUMBER;
        IF (J<1) OR (J>7) THEN FLAG2:=TRUE;
      UNTIL FLAG2=FALSE;
      WRITELN(CHR(12));
      CASE J OF
        1: NMETC1;
        2: NMETC2;
        3: NMETC3;
        4: NMETC4;
        5: NMETC5;
        6: NMETC6;
        7: NMETC7;
      END;
    END;
  END;
END;

```

PROCEDURE METC8;

```
BEGIN
  WRITE('      MODIFICATION OF ');
  FOR K:=1 TO 15 DO WRITE(SP[I,K]);
  ERROR:=TRUE;
  WHILE ERROR=TRUE DO
    BEGIN
      LF(3);
      WRITE(' CHANGE VALUE FOR WHAT ION NUMBER?: ');
      INCHAR;
      IF (NUMBER<1) OR (NUMBER>NION) THEN ERROR:=TRUE;
      END;
    K:=NUMBER;
    LF(2);
    WRITELN(' CURRENT VALUE IS ',ION[K,I]:2);
    ERROR:=TRUE;
    WHILE ERROR=TRUE DO
      BEGIN
        LF(1);
        WRITE(' DESIRED VALUE: ');
        INCHAR;
        END;
      ION[K,I]:=NUMBER;
    END;
  END;
```

PROCEDURE METC7;

```
BEGIN
  WRITE('      MODIFICATION OF NUMBER OF HYDROGEN ATOMS FOR ');
  FOR K:=1 TO 15 DO WRITE(SP[I,K]);
  LF(3);
  WRITELN(' CURRENT NAME IS ',HYDRO[I]:3);
  ERROR:=TRUE;
  WHILE ERROR=TRUE DO
    BEGIN
      LF(1);
      WRITE(' DESIRED VALUE: ');
      INCHAR;
      END;
    HYDRO[I]:=NUMBER;
  END;
```

PROCEDURE METC6;

```
BEGIN
  WRITE('      MODIFICATION OF NUMBER OF OXYGEN ATOMS FOR ');
  FOR K:=1 TO 15 DO WRITE(SP[I,K]);
  LF(3);
  WRITELN(' CURRENT VALUE IS ',OXYGEN[I]:3);
  ERROR:=TRUE;
  WHILE ERROR=TRUE DO
    BEGIN
      LF(1);
      WRITE(' DESIRED VALUE: ');
      INCHAR;
      END;
    OXYGEN[I]:=NUMBER;
  END;
```

PROCEDURE METC5;

```
BEGIN
  WRITE('      MODIFICATION OF NUMBER OF METAL ATOMS FOR ');
  FOR K:=1 TO 15 DO WRITE(SP[I,K]);
  LF(3);
  WRITELN(' CURRENT VALUE IS ',METAL[I]:3);
  ERROR:=TRUE;
  WHILE ERROR=TRUE DO
    BEGIN
      LF(1);
      WRITE(' DESIRED VALUE: ');
      INCHAR;
      END;
    METAL[I]:=NUMBER;
  END;
```

```

PROCEDURE METC4;
BEGIN
  WRITE('      MODIFICATION OF CHARGE FOR ');
  FOR K:=1 TO 15 DO WRITE(SP(I,K));
  LF(3);
  WRITELN(' CURRENT VALUE IS ',Z(I):2);
  ERROR:=TRUE;
  WHILE ERROR=TRUE DO
    BEGIN
      LF(1);
      WRITE(' DESIRED VALUE: ');
      INCHAR;
    END;
    Z(I):=NUMBER;
  END;
END;

PROCEDURE METC3;
BEGIN
  WRITE('      MODIFICATION OF ACTIVITY FOR ');
  FOR K:=1 TO 15 DO WRITE(SP(I,K));
  LF(3);
  WRITELN(' CURRENT VALUE IS ',AM(I):2:6);
  ERROR:=TRUE;
  WHILE ERROR=TRUE DO
    BEGIN
      LF(1);
      WRITE(' DESIRED VALUE: ');
      INREAL;
    END;
    AM(I):=RNUMBER;
  END;
END;

PROCEDURE METC2;
BEGIN
  WRITE('      MODIFICATION OF FREE ENERGY FOR ');
  FOR K:=1 TO 15 DO WRITE(SP(I,K));
  LF(3);
  WRITELN(' CURRENT VALUE IS ',F(I):10:2);
  ERROR:=TRUE;
  WHILE ERROR=TRUE DO
    BEGIN
      LF(1);
      WRITE(' DESIRED VALUE: ');
      INREAL;
    END;
    F(I):=RNUMBER;
  END;
END;

PROCEDURE METC1;
BEGIN
  WRITELN('      MODIFICATION OF SPECIE NAME');
  LF(3);
  WRITE(' CURRENT NAME IS ');
  FOR K:=1 TO 15 DO WRITE(SP(I,K));
  LF(2);
  WRITE(' DESIRED VALUE: ');
  FOR K:=1 TO 15 DO SP(I,K):=' ';
  M:=1;
  GETMET;
END;

```

```

PROCEDURE METCOR;
VAR FLAG1:BOOLEAN;
BEGIN
  ERROR:=TRUE;
  WHILE ERROR=TRUE DO
    BEGIN
      LF(1);
      WRITE(' ENTER METALLIC SPECIE NUMBER: ');
      INCHAR;
      IF (NUMBER(1) OR (NUMBER)N) THEN ERROR:=TRUE;
    END;
  I:=NUMBER;
  REPEAT
    FLAG1:=FALSE;
    LF(2);
    WRITELN(' PARAMETER TO BE MODIFIED -');
    LF(1);
    WRITELN('      1 - SPECIES NAME');
    WRITELN('      2 - FREE ENERGY OF FORMATION');
    WRITELN('      3 - ACTIVITY');
    WRITELN('      4 - CHARGE');
    WRITELN('      5 - NUMBER OF METAL ATOMS');
    WRITELN('      6 - NUMBER OF OXYGEN ATOMS');
    WRITELN('      7 - NUMBER OF HYDROGEN ATOMS');
    WRITELN('      8 - NUMBER OF CHARACTERISTIC ATOMS');
    ERROR:=TRUE;
    WHILE ERROR=TRUE DO
      BEGIN
        LF(1);
        WRITE(' ENTER OPTION: ');
        INCHAR;
      END;
      J:=NUMBER;
      IF (J(1) OR (J)8) THEN FLAG1:=TRUE;
    UNTIL FLAG1=FALSE;
    WRITELN(CHR(12));
    CASE J OF
      1: METC1;
      2: METC2;
      3: METC3;
      4: METC4;
      5: METC5;
      6: METC6;
      7: METC7;
      8: METC8;
    END;
  END;
END;

PROCEDURE TEMPCOR;
BEGIN
  WRITELN(' CURRENT TEMPERATURE VALUE IS ',T:6:2,' DEGREES KELVIN');
  ERROR:=TRUE;
  WHILE ERROR=TRUE DO
    BEGIN
      LF(1);
      WRITE(' DESIRED VALUE: ');
      INREAL;
    END;
  T:=RNUMBER;
END;

```



```

PROCEDURE FECOR;
BEGIN
  WRITELN(' CURRENT FREE ENERGY IS ',FEH2O:8:2,' CALS/MOLE');
  ERROR:=TRUE;
  WHILE ERROR=TRUE DO
    BEGIN
      LF(1);
      WRITE(' DESIRED VALUE: ');
      INREAL;
    END;
    FEH2O:=RNUMBER;
  END;

PROCEDURE DATACORRECT;
VAR OPT:CHAR;
BEGIN
  WRITELN(CHR(12));
  REPEAT
    WRITELN(CHR(12));
    LF(1);
    WRITELN(' MODIFY WHICH VALUE?');
    LF(1);
    WRITELN('      1 - TEMPERATURE');
    WRITELN('      2 - FREE ENERGY OF H2O');
    WRITELN('      3 - NON-METALLIC ION DATA');
    WRITELN('      4 - METALLIC SPECIES DATA');
    WRITELN('      5 - ALL DATA IS NOW CORRECT');
    LF(1);
    WRITE(' ENTER OPTION: ');
    READLN(OPT);
    WRITELN(CHR(12));
    CASE OPT OF
      '1': TEMPCOR;
      '2': FECOR;
      '3': NONMETCOR;
      '4': METCOR;
      '5': OPT:='N';
    END;
    LF(2);
  UNTIL OPT='N';
END;

BEGIN
END.

```

USER'S GUIDE FOR THE
INTERACTIVE PH - POTENTIAL PROGRAM

This introductory guide should be read prior to operation
of the program.

"When all else fails, push the reset button..."

When the reset button fails, pull the plug..."

Eginhard Muth

INTRODUCTION

The microcomputer version of the PH - POTENTIAL PROGRAM is easy to use, even for those with little or no computer experience. This guide explains, in simple terms, how to get started and what the operator must do to use the program effectively.

GETTING STARTED

Getting started is easy. Simply place the diskettes in the proper disk drives and turn on the power. The program will begin execution automatically. The following explains the process in detail.

- 1 - Open disk drive #1. Insert the diskette labeled POURBAIX 1 into disk drive #1. (For the beginner, hold the diskette in either hand, palm up, and with your thumb on the label, gently slide in the diskette and close the disk drive door.)

- 2 - Repeat step 1 for disk drive #2 and the diskette labeled POURBAIX 2.

NOTE: For single drive systems, the program can be executed with only POURBAIX 1.

- 3 - Turn on the power for the computer. If the power was already on turn the computer off and then on again. The disk drives will make whirring noises as the computer prepares for operation. In just a few seconds, the program will begin execution automatically and prompt for inputs.

ENTERING THE DATA

The program sequentially prompts for the required data. Simply type in the name or number as asked. If the computer responds with "IMPROPER NUMBER" see Appendix 1 for possible causes.

Data to be Entered (R = Real, I = Integer, C = Character.)

- 1 - TEMPERATURE (degrees Kelvin). (R)
- 2 - GIBB'S FREE ENERGY OF FORMATION OF H₂O AT THE TEMPERATURE BEING CONSIDERED (in calories per mole). (R)
- 3 - NUMBER OF NON-METALLIC IONS CONSIDERED. (I)

For each non-metallic ionic species considered:

- 4A - NAME OF NON-METALLIC ION. (C)
- 4B - FREE ENERGY OF FORMATION (in calories per mole). (R)
- 4C - THERMODYNAMIC ACTIVITY. (R)
- 4D - ELECTRICAL CHARGE. (I)
- 4E - NUMBER OF CHARACTERISTIC ATOMS (atoms other than oxygen or hydrogen). (I)
- 4F - NUMBER OF OXYGEN ATOMS IN THE IONIC SPECIES. (I)
- 4G - NUMBER OF HYDROGEN ATOMS IN THE IONIC SPECIES. (I)
- 5 - NUMBER OF METALLIC SPECIES CONSIDERED. (I)

For each metallic species considered:

- 6A - NAME OF METALLIC SPECIES. (C)
- 6B - GIBB'S FREE ENERGY OF FORMATION (calories per mole). (R)
- 6C - THERMODYNAMIC ACTIVITY. (R)
- 6D - ELECTRICAL CHARGE. (I)
- 6E - NUMBER OF METAL ATOMS IN THE SPECIES. (I)
- 6F - NUMBER OF OXYGEN ATOMS. (I)
- 6G - NUMBER OF HYDROGEN ATOMS. (I)
- 6H - NUMBER OF CHARACTERISTIC ATOMS OF IONIC SPECIES #1,
2, 3, etc. (I)

PROGRAM EXECUTION

Execution of the program begins with the last piece of data entered. The following message will appear on the screen:

MODIFY THE DATA ? [Y/N]:

Type N if the data was entered correctly or if you want to see the data before modification.

Typing Y will start the data modification routine. The computer will then display the following menu:

MODIFY WHICH VALUE ?

- 1 - TEMPERATURE
- 2 - FREE ENERGY OF H2O
- 3 - NON-METALLIC ION DATA
- 4 - METALLIC SPECIES DATA
- 5 - ALL DATA IS NOW CORRECT

ENTER OPTION:

For options 1 and 2, the old values are displayed along with a prompt for the desired value. For options 3 and 4, the computer prompts for the parameter to be modified before displaying the old value and awaiting input of the new value. Once a value has been modified, the "MODIFY WHICH VALUE ?" menu is again displayed. Option 5 will end the data modification routine.

The computer will next prompt with:

DISPLAY TABULATED DATA ? [Y/N]:

Type N if you do not want to see the data displayed in tabular form.

Typing Y will start the data display routine. The computer prompts with:

DATA DISPLAY OPTIONS

P - PRINTER

T - TERMINAL

ENTER OPTION:

The data is then displayed as specified.

APPLE NOTE: To temporarily halt execution of the program type (CTRL) S ; that is type S while depressing the CTRL key. This freezes the screen display until (CTRL) S is typed again.

The computer next prompts with:

EQUATION LISTING OPTIONS

P - PRINTER

T - TERMINAL

ENTER OPTION:

The equations will be listed as specified.

The computer displays the message "EXECUTION COMPLETE...." to signal the end of the run and prompts with:

EXECUTE AGAIN ? [Y/N]:

Type N to quit.

Type Y and the computer asks:

REPEAT EXECUTION WITH SAME DATA ? [Y/N]:

Type N and the computer asks:

MODIFY CURRENT DATA SET ? [Y/N]:

Type Y to initiate the data modification routine.

Type N and the system reinitializes and prompts for new inputs.

APPENDIX 1

REASONS FOR "IMPROPER DATA" MESSAGE

1 - Entering an alphabetic character for a numeric variable.

Retype the number correctly.

2 - A decimal point (.) for an integer variable.

Retype the number omitting the decimal point.

3 - A plus sign (+) for electric charge.

Retype the number omitting the plus sign.

Note: Negative values do require the minus sign.

PROGRAMMING NOTES

The interactive version of the PH - POTENTIAL PROGRAM is largely a translation of the WATFIV version that makes use of UCSD - APPLE PASCAL features. Despite the limitations imposed on the size of procedures and the limitations imposed by the stack, the program is designed in modules to facilitate modification and/or extensions. The program is intended to be implementable on any microcomputer that supports the UCSD operating system.

The current version makes extensive use of Intrinsic Units, separately compiled program segments that have been installed into the SYSTEM.LIBRARY. These Units are swapped into active memory only when a call is made to a procedure found in the Unit. A brief description of each of the Units follows.

GETVAL

This Unit converts an integer, $CC[j]$, into a corresponding character array, $SAVE$. For example, a $CC[j]$ value of 123 is converted to the array of values $SAVE[1]='1'$, $SAVE[2]='2'$, $SAVE[3]='3'$.

CONVERT

This Unit converts character arrays to integer or real values through the procedures $CHARTOINT$ and $CHARTOREAL$.

INDATA

This Unit contains the data entry and data modification routines. All inputs are read as characters to prevent crashing by variable type mismatches. Integer and real values are extracted by the $CONVERT$ Unit.

STABLE

This Unit calculates the areas of predominance for the species being considered.

 * TEMPERATURE = 298.15 *

ION NUMBER	IONIC SPECIES	FREE ENERGY OF FORMATION	IONIC ACTIVITY	CHARGE
1	CL-	-31372.0	0.100000	-1
2	HS-	2880.0	0.100000	-1

ION NUMBER	CHARACTERISTIC ATOMS	OXYGEN ATOMS	HYDROGEN ATOMS
1	1	0	0
2	1	0	1

METALLIC SPECIES	FREE ENERGY OF FORMATION	SPECIES ACTIVITY	CHARGE
FE	0.0	1.000000	0
FE3O4	-242700.	1.000000	0
FE2O3	-177400.	1.000000	0
HFE02-	-90300.0	0.0000001	-1
FE0H++	-54830.0	0.0000001	2
FE(OH)2+	-104700.	0.0000001	1
FECL2(AQ)	-81590.0	0.0000001	0
FECL++	-34400.0	0.0000001	2
FES(SOL)	-24000.0	1.000000	0
FES2(SOL)	-39900.0	1.000000	0
	-196820.	0.0000001	0

METALLIC SPECIES	METAL ATOMS	OXYGEN ATOMS	HYDROGEN ATOMS
FE	1	0	0
FE3O4	3	4	0
FE2O3	2	3	0
HFE02-	1	2	1
FE0H++	1	1	1
FE(OH)2+	1	2	2
FECL2(AQ)	1	0	0
FECL++	1	0	0
FES(SOL)	1	0	0
FES2(SOL)	1	0	0
	1	4	0

METALLIC SPECIES	NUMBER OF CHARACTERISTIC ATOMS OF EACH IONIC SPECIES				
	ION1	ION2	ION3	ION4	ION5
FE	0	0			
FE3O4	0	0			
FE2O3	0	0			
HFE02-	0	0			
FE0H++	0	0			
FE(OH)2+	0	0			
FECL2(AQ)	2	0			
FECL++	1	0			
FES(SOL)	0	1			
FES2(SOL)	0	2			
	0	1			

NUMBER	EQUILIBRIUM	BALANCED CHEMICAL EQUATION
1	$E = -0.0864 - 0.0592\text{PH}$	$3\text{FE} + 4\text{H}_2\text{O} = \text{FE}_3\text{O}_4 + 8\text{H}^+ + 8\text{E}^-$
2	$E = -0.0530 - 0.0592\text{PH}$	$2\text{FE} + 3\text{H}_2\text{O} = \text{FE}_2\text{O}_3 + 6\text{H}^+ + 6\text{E}^-$
3	$E = 0.3229 - 0.0887\text{PH}$	$\text{FE} + 2\text{H}_2\text{O} = \text{HFE}^+\text{O}_2^- + 3\text{H}^+ + 2\text{E}^-$
4	$E = -0.0914 - 0.0197\text{PH}$	$\text{FE} + \text{H}_2\text{O} = \text{FE}^+\text{OH} + \text{H}^+ + 3\text{E}^-$
5	$E = 0.0071 - 0.0394\text{PH}$	$\text{FE} + 2\text{H}_2\text{O} = \text{FE}(\text{OH})_2^+ + 2\text{H}^+ + 3\text{E}^-$
6	$E = -0.5270$	$\text{FE} + 2\text{CL}^- = \text{FECL}_2(\text{AQ}) + 2\text{E}^-$
7	$E = -0.1424$	$\text{FE} + \text{CL}^- = \text{FECL}^{++} + 3\text{E}^-$
8	$E = -0.5532 - 0.0296\text{PH}$	$\text{FE} + \text{HS}^- = \text{FES}(\text{SOL}) + \text{H}^+ + 2\text{E}^-$
9	$E = -0.4654 - 0.0296\text{PH}$	$\text{FE} + 2\text{HS}^- = \text{FES}_2(\text{SOL}) + 2\text{H}^+ + 4\text{E}^-$
10	$E = 0.0878 - 0.0532\text{PH}$	$\text{FE} + 4\text{H}_2\text{O} + \text{HS}^- = 9\text{H}^+ + 10\text{E}^-$
11	$E = 0.2144 - 0.0592\text{PH}$	$2\text{FE}_3\text{O}_4 + \text{H}_2\text{O} = 3\text{FE}_2\text{O}_3 + 2\text{H}^+ + 2\text{E}^-$
12	$E = -1.3144 + 0.0296\text{PH}$	$3\text{HFE}^+\text{O}_2^- - 2\text{H}_2\text{O} = \text{FE}_3\text{O}_4 - \text{H}^+ + 2\text{E}^-$
13	$E = -0.1318 + 0.2958\text{PH}$	$\text{FE}_3\text{O}_4 - \text{H}_2\text{O} = 3\text{FE}^+\text{OH} + 5\text{H}^+ + \text{E}^-$
14	$E = 0.7555 + 0.1183\text{PH}$	$\text{FE}_3\text{O}_4 + 2\text{H}_2\text{O} = 3\text{FE}(\text{OH})_2^+ - 2\text{H}^+ + \text{E}^-$
15	$E = 1.2353 - 0.2367\text{PH}$	$3\text{FECL}_2(\text{AQ}) + 4\text{H}_2\text{O} - 6\text{CL}^- = \text{FE}_3\text{O}_4 + 8\text{H}^+ + 2\text{E}^-$
16	$E = -0.5902 + 0.4733\text{PH}$	$\text{FE}_3\text{O}_4 - 4\text{H}_2\text{O} + 3\text{CL}^- = 3\text{FECL}^{++} - 8\text{H}^+ + \text{E}^-$
17	$E = 1.3141 - 0.1479\text{PH}$	$3\text{FES}(\text{SOL}) + 4\text{H}_2\text{O} - 3\text{HS}^- = \text{FE}_3\text{O}_4 + 5\text{H}^+ + 2\text{E}^-$
18	$E = -1.2235 + 0.0296\text{PH}$	$\text{FE}_3\text{O}_4 - 4\text{H}_2\text{O} + 6\text{HS}^- = 3\text{FES}_2(\text{SOL}) - 2\text{H}^+ + 4\text{E}^-$
19	$E = 0.1511 - 0.0511\text{PH}$	$\text{FE}_3\text{O}_4 + 8\text{H}_2\text{O} + 3\text{HS}^- = 3\text{H}^+ + 19\text{H}^+ + 22\text{E}^-$
20	$E = -0.8048$	$2\text{HFE}^+\text{O}_2^- - \text{H}_2\text{O} = \text{FE}_2\text{O}_3 + 2\text{E}^-$
21	$\text{PH} = 0.98$	$2\text{FE}^+\text{OH} + \text{H}_2\text{O} = \text{FE}_2\text{O}_3 + 4\text{H}^+$
22	$\text{PH} = -3.05$	$2\text{FE}(\text{OH})_2^+ - \text{H}_2\text{O} = \text{FE}_2\text{O}_3 + 2\text{H}^+$

23	E= 0.8950 - 0.1775PH	$2*FECL_2(AQ) + 3*H_2O - 4*CL^- =$ $FE_2O_3 + 6*H^+ + 2*E^-$
24	PH= 1.51	$2*FECL_{++} + 3*H_2O - 2*CL^- =$ $FE_2O_3 + 6*H^+$
25	E= 0.9476 - 0.1183PH	$2*FES(SOL) + 3*H_2O - 2*HS^- =$ $FE_2O_3 + 4*H^+ + 2*E^-$
26	E= -1.7028 + 0.0592PH	$FE_2O_3 - 3*H_2O + 4*HS^- =$ $2*FES_2(SOL) - 2*H^+ + 2*E^-$
27	E= 0.1481 - 0.0507PH	$FE_2O_3 + 5*H_2O + 2*HS^- =$ $2* + 12*H^+ + 14*E^-$
28	E= -0.9202 + 0.1183PH	$HFeO_2^- - H_2O =$ $FeOH_{++} - 2*H^+ + E^-$
29	E= -0.6245 + 0.0592PH	$HFeO_2^- =$ $Fe(OH)_2 + - H^+ + E^-$
30	PH= 9.58	$FECL_2(AQ) + 2*H_2O - 2*CL^- =$ $HFeO_2^- + 3*H^+$
31	E= -1.0730 + 0.1775PH	$HFeO_2^- - 2*H_2O + CL^- =$ $FECL_{++} - 3*H^+ + E^-$
32	PH= 14.81	$FES(SOL) + 2*H_2O - HS^- =$ $HFeO_2^- + 2*H^+$
33	E= -1.2538 + 0.0296PH	$HFeO_2^- - 2*H_2O + 2*HS^- =$ $FES_2(SOL) - H^+ + 2*E^-$
34	E= 0.0290 - 0.0444PH	$HFeO_2^- + 2*H_2O + HS^- =$ $+ 6*H^+ + 8*E^-$
35	PH= 5.00	$FeOH_{++} + H_2O =$ $Fe(OH)_2 + H^+$
36	E= 0.7796 - 0.0592PH	$FECL_2(AQ) + H_2O - 2*CL^- =$ $FeOH_{++} + H^+ + E^-$
37	PH= 2.58	$FECL_{++} + H_2O - CL^- =$ $FeOH_{++} + H^+$
38	E= 0.8322	$FES(SOL) + H_2O - HS^- =$ $FeOH_{++} + E^-$
39	E= -1.5874 - 0.0592PH	$FeOH_{++} - H_2O + 2*HS^- =$ $FES_2(SOL) + H^+ + E^-$
40	E= 0.1646 - 0.0676PH	$FeOH_{++} + 3*H_2O + HS^- =$ $+ 8*H^+ + 7*E^-$
41	E= 1.0753 - 0.1183PH	$FECL_2(AQ) + 2*H_2O - 2*CL^- =$ $Fe(OH)_2 + 2*H^+ + E^-$
42	PH= 3.79	$FECL_{++} + 2*H_2O - CL^- =$ $Fe(OH)_2 + 2*H^+$
43	E= 1.1279 - 0.0592PH	$FES(SOL) + 2*H_2O - HS^- =$ $Fe(OH)_2 + H^+ + E^-$
44	E= -1.8831	$Fe(OH)_2 - 2*H_2O + 2*HS^- =$ $FES_2(SOL) + E^-$
45	E= 0.1223 - 0.0592PH	$Fe(OH)_2 + 2*H_2O + HS^- =$ $+ 7*H^+ + 7*E^-$
46	E= 0.6268	$FECL_2(AQ) - CL^- =$ $FECL_{++} + E^-$

47	PH= -0.89	FECL2(AQ) - 2*CL- + HS- = FES(SOL) + H+
48	E= -0.4039 - 0.0592PH	FECL2(AQ) - 2*CL- + 2*HS- = FES2(SOL) + 2*H+ + 2*E-
49	E= 0.2414 - 0.0666PH	FECL2(AQ) + 4*H2O - 2*CL- + HS- = + 9*H+ + 8*E-
50	E= 0.6794 + 0.0592PH	FES(SOL) + CL- - HS- = FECL++ - H+ + E-
51	E= -1.4346 - 0.1183PH	FECL++ - CL- + 2*HS- = FES2(SOL) + 2*H+ + E-
52	E= 0.1864 - 0.0761PH	FECL++ + 4*H2O - CL- + HS- = + 9*H+ + 7*E-
53	E= -0.3776 - 0.0296PH	FES(SOL) + HS- = FES2(SOL) + H+ + 2*E-
54	E= 0.2480 - 0.0592PH	FES(SOL) + 4*H2O = + 8*H+ + 8*E-
55	E= 0.4566 - 0.0690PH	FES2(SOL) + 4*H2O - HS- = + 7*H+ + 6*E-

* AREA OF PREDOMINANCE FOR: FE *

NO LOWER LIMIT

POTENTIAL 1	PH 1	POTENTIAL 2	PH 2	LINE NO.
-0.527	-2.00	-0.527	-0.89	6
-0.527	-0.89	-0.991	14.81	8
-0.991	14.81	-1.097	16.00	3
MINIMUM PH = -2.00				
MAXIMUM PH = 16.00				

* AREA OF PREDOMINANCE FOR: FE3O4 *

POTENTIAL 1	PH 1	POTENTIAL 2	PH 2	LINE NO.
-0.801	14.30	-0.750	16.00	18
-0.801	14.30	-0.876	14.81	17
-0.876	14.81	-0.841	16.00	12
-0.750	16.00	-0.841	16.00	

* AREA OF PREDOMINANCE FOR: FE2O3 *

NO AREA OF PREDOMINANCE

* AREA OF PREDOMINANCE FOR: HFEO2- *

POTENTIAL 1	PH 1	POTENTIAL 2	PH 2	LINE NO.
-0.876	14.81	-0.841	16.00	17
-0.991	14.81	-1.097	16.00	3
-0.876	14.81	-0.991	14.81	32
-0.841	16.00	-1.097	16.00	

* AREA OF PREDOMINANCE FOR: FEOH++ *

NO AREA OF PREDOMINANCE

* AREA OF PREDOMINANCE FOR: FE(OH)2+ *

NO AREA OF PREDOMINANCE

* AREA OF PREDOMINANCE FOR: FECL2(AQ) *

POTENTIAL 1	PH 1	POTENTIAL 2	PH 2	LINE NO.
-0.286	-2.00	-0.351	-0.89	48
-0.527	-2.00	-0.527	-0.89	6
-0.286	-2.00	-0.527	-2.00	
-0.351	-0.89	-0.527	-0.89	47

* AREA OF PREDOMINANCE FOR: FECL++ *

NO AREA OF PREDOMINANCE

* AREA OF PREDOMINANCE FOR: FES(SOL) *

POTENTIAL 1	PH 1	POTENTIAL 2	PH 2	LINE NO.
-0.351	-0.89	-0.801	14.30	53
-0.801	14.30	-0.876	14.81	17
-0.527	-0.89	-0.991	14.81	8
-0.351	-0.89	-0.527	-0.89	47
-0.876	14.81	-0.991	14.81	32

* AREA OF PREDOMINANCE FOR: FES2(SOL) *

POTENTIAL 1	PH 1	POTENTIAL 2	PH 2	LINE NO.
0.595	-2.00	-0.648	16.00	55
-0.286	-2.00	-0.351	-0.89	48
-0.351	-0.89	-0.801	14.30	53
-0.801	14.30	-0.750	16.00	18
0.595	-2.00	-0.285	-2.00	
-0.648	16.00	-0.750	16.00	

* AREA OF PREDOMINANCE FOR: *

NO UPPER LIMIT

POTENTIAL 1	PH 1	POTENTIAL 2	PH 2	LINE NO.
0.595	-2.00	-0.648	16.00	55

MINIMUM PH = -2.00
MAXIMUM PH = 16.00

* AREA OF PREDOMINANCE FOR: HFEO2- * DISSOLVED SPECIES DIAGRAM

NO LOWER LIMIT

POTENTIAL 1	PH 1	POTENTIAL 2	PH 2	LINE NO.
-0.396	9.58	-0.681	16.00	34

MINIMUM PH = 9.58 LINE NO. 30
MAXIMUM PH = 16.00

* AREA OF PREDOMINANCE FOR: FeOH++ * DISSOLVED SPECIES DIAGRAM

NO AREA OF PREDOMINANCE

* AREA OF PREDOMINANCE FOR: Fe(OH)2+ * DISSOLVED SPECIES DIAGRAM

NO AREA OF PREDOMINANCE

* AREA OF PREDOMINANCE FOR: FeCl2(AQ) * DISSOLVED SPECIES DIAGRAM

NO LOWER LIMIT

POTENTIAL 1	PH 1	POTENTIAL 2	PH 2	LINE NO.
0.375	-2.00	-0.396	9.58	49

MINIMUM PH = -2.00
MAXIMUM PH = 9.58 LINE NO. 30

* AREA OF PREDOMINANCE FOR: FeCl++ * DISSOLVED SPECIES DIAGRAM

NO AREA OF PREDOMINANCE

* AREA OF PREDOMINANCE FOR: * DISSOLVED SPECIES DIAGRAM

NO UPPER LIMIT

POTENTIAL 1	PH 1	POTENTIAL 2	PH 2	LINE NO.
0.375	-2.00	-0.396	9.58	49
-0.396	9.58	-0.681	16.00	34

MINIMUM PH = -2.00
MAXIMUM PH = 16.00

DATE
ILME